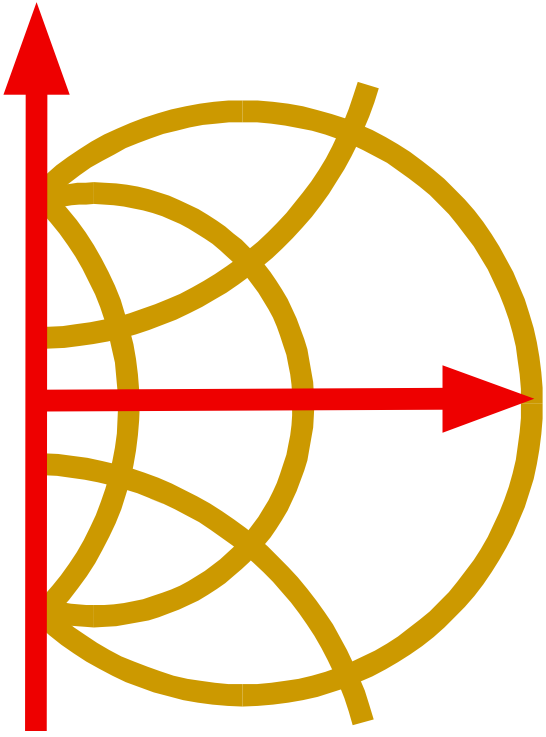
ESSENTIAL MACLEOD

Optical Coating Design Program



USER'S MANUAL

Information in this document is subject to change without notice and does not represent a commitment on the part of Thin Film Center Inc. The software described in this document is furnished under a license agreement. The software may be used or copied only in accordance with the terms of the agreement.

Version 11.8

Thin Film Center Inc
2745 E Via Rotunda
Tucson AZ 85716, USA
Tel: +1 520 322 6171
Email: info@thinfilmcenter.com
Web: thinfilmcenter.com

THIN FILM CENTER INC

ESSENTIAL MACLEOD SOFTWARE LICENSE AGREEMENT

SINGLE USER

The software in the Macleod package and the material in the accompanying manual are protected by United States copyright law and by international treaty provisions.
The software itself continues to be the property of Thin Film Center Inc who retain ownership and all rights, including copyright. The purchaser is purchasing a license to use the software and owns only the physical media on which the program is supplied.
Copying of any part of the package or manual is strictly forbidden except that the Licensee may load the package into a computer in order to make use of it, may make a print copy of the on-line manual for his or her own use, and may make archival copies of the package for safe keeping.
The Licensee is limited to having the package in use in only one piece of single-user computer hardware at any one time.
The package may not be exported nor reexported nor transferred except as permitted by the laws and regulations of the United States of America.
We have used our best efforts to make the package run correctly and to be as versatile and useful as possible. Nevertheless the package is provided "as is" without warranty of any kind other than the replacement of defective disks or physical documentation as described above. The entire risk as to the results and performance of the package is assumed by the Licensee along with the entire cost of servicing, repair or correction.
Furthermore no representation is made regarding either the use or the results of the use of the package in any terms including accuracy, reliability or correctness. In no event shall Thin Film Center Inc or any of its employees or associates be held liable for damages, including but not limited to, special or consequential damages, arising from use of the package.
Use of the package implies acceptance of these terms.

Note:
We ask that the Licensee designate a User for the package and that the User be registered with us. Support for the package is provided to the registered User only. We permit the User to have the package installed on more than one computer, for example a laptop and/or a computer at home. We permit casual use of the program by other people but where the use is likely to exceed single-user level we ask that a license be obtained for each additional user. Please request details of our Terms and Conditions for Multiple Users.

TABLE OF CONTENTS

ESSENTIAL MACLEOD OPTICAL COATING DESIGN AND ANALYSIS PROGRAM

FOR THE
MICROSOFT® WINDOWS® OPERATING SYSTEM

INTRODUCTION

This manual describes the version of the Essential Macleod Thin-Film Design Package for the Microsoft® Windows® Operating System.

Familiarity with the Microsoft Windows Operating System is assumed throughout the manual. In particular mouse actions like selection, dragging, clicking and so on will be used without further explanation. Where keystrokes are concerned, the notation **<Enter>** or **<Return>** is used to mean "press the key marked Enter (or Return)" similarly for **<Ctrl>** and **<Esc>. <Fl>, <F2>** etc. refer to the function keys.

About The Program

The Essential Macleod program contains all the essentials for the design and performance calculation of optical coatings. In particular it will calculate a wide range of performance parameters of a given coating design including the usual reflectance and transmittance magnitude and phase, but also color, ultrafast, ellipsometric quantities and from the zero'th up to the third derivative as a function of wavelength. It will estimate the effects of random errors in the layers. It will refine existing designs to improve their performance and it will synthesize designs that start with virtually no instructions other than the materials to be used and the performance that is targeted. It includes allowance for layer packing density. It has powerful design editors to make it very easy to create or change even the most complex designs. It also maintains the files that contain the optical constants of materials. The Essential Macleod will also calculate performance of series of different substrates, with or without associated coatings and it will perform a wide range of analytical functions such as generating admittance diagrams and electric field distributions. It has a completely flexible system of variable units.

The Essential Macleod is equipped to export coating designs to the Zemax, Code V, FRED, and VirtualLab optical design packages. It will also export performance to the LinkSIM simulation tool.

Optional enhancements add a virtually limitless range of possible performance functions, run sheets and monitoring curves with links to thin film monitors.

The package is an integrated whole with the operation controlled almost entirely from menus. The menu commands are designed to permit the user to indicate *what* has to be done without needing to indicate *how*. To calculate an aspect of performance, for example, the user simply tells the package to produce a plot or a table. The underlying operation and organization is completely automatic. The description that follows,

therefore, concentrates on the menu commands, what they are and what they do. It is purely a description of the operation of the software package. It does not go into details of the calculation techniques nor does it discuss design technique.

The Essential Macleod uses a Multiple Document Interface (MDI). A document can be a plot, a table, a design, a list of materials and so on. Multiple Document Interface means that many documents may be displayed at once. One document at a time is active. The menu bar changes as the active document changes so that the menu commands always apply to whichever of the open documents is the active one. For example, if a plot is active then the Edit menu will apply to the plot and will permit such things as changing the parameters of the axes. The user will find that it is often useful to be able to keep several designs open simultaneously. Should the capacity of Windows or of the computer be exceeded then the user will simply be requested to reduce the number of open documents. There is no need constantly to keep track of what is open. We do recommend, however, that unnecessary documents should be closed to avoid clutter.

Throughout the operation of the package, designs and specifications are saved to various files. The principal files are known as design files and they contain not just the sequence of layers but also their materials and the calculation parameters that should be used to evaluate the design. If a design is passed to refinement, the refinement specification also becomes part of the design file. The operation of saving the design and parameters can be manually performed at any time by choosing the appropriate menu item but it is also automatically initiated at those stages where there is a danger that something might otherwise be lost. In spite of this automatic feature, we do recommend that the user acquire the habit of saving the work at intervals. In particular when moving from one design to another it often seems convenient just to write the new design over the old. However, if the existing design is important the editing process will change it perhaps beyond recovery. No automatic save is initiated whenever a design is edited - editing is a very simple and straightforward process. Before beginning major editing, where a design is going to be substantially altered, it is good practice to save the design twice, once in the existing design file, thereby preserving the current design for later recall, and once in a new design file, which can then be edited without fear of changing the original. You may find this approach useful in other applications such as word processors also. Should it happen that something was overwritten when it should not, there are powerful Undo and Redo commands that can help.

In the Essential Macleod the optical constant information for the thin film materials is kept in separate files in one or more materials databases. In the designs, the materials of the films and substrate are referred to explicitly by name (normally the chemical formula). A material database consists of a set of materials files together with control files that are kept in a separate folder, the path being the identifier for the database. Many different material databases may exist together. This is a particularly useful feature of the Essential Macleod and we encourage the user to make full use of it. Separate databases could be used, for example, for infrared materials as distinct from visible materials with wavelength stated in microns rather than nanometres. Alternatively, different databases could be used for different customers or for different plants or processes. In order to keep track of the particular database that was used to generate a design, information on both the database and the number/name conversion for the materials used, is stored in each design file. This information is compared with the existing database when a design file is read and only if an exact match is found can the calculations proceed without

intervention. The material database can easily be changed but only when there are no open documents. The **General** command in the **Options** menu opens the form that contains the necessary command for changing the material database. A number of facilities are provided to simplify the maintenance of many different material databases. These are described later in the manual. A comprehensive searchable list of materials is provided in the Materials Library.

Then further help in organization is provided by the Jobs facility. This permits all files, materials and references as well as designs to be kept separately in a designated folder that can be removed to an archive when the particular task is complete.

INSTALLATION

If the Essential Macleod program has already been correctly installed on the hard disk of the computer, you can skip this section on first reading, returning to it later if you want to alter the configuration data. However, if you are loading the Essential Macleod program for the first time you should read the section carefully.

System Requirements

The program is fully compatible with Microsoft® supported versions of the Windows® operating system. Although the space actually taken up by the program is much less, we recommend that some 20-25Mb of hard disk storage should be available. As the program is used, it is inevitable, and desirable, that design files, data files, text files and specifications will multiply.

License System

The Essential Macleod has a built-in licensing system that operates invisibly once authorization is obtained. The procedure for obtaining a full license is described in detail at the end of this manual. The Macleod software is licensed automatically for an initial period of 15 days to allow use of the software immediately on installation and to allow time to obtain the full license. It is possible to obtain the license via fax, e-mail or telephone and the procedure is simply an exchange of information. The customer must provide a Site Code to Thin Film Center. Thin Film Center then issues a Site Key to the customer which allows full licensing of the Macleod software to occur. These codes are simple alphanumeric strings. Note that with a transferrable license, transferring the license from one machine to another is very straightforward.

Installing the Software

Make sure that you are logged on with Administrator privileges. The taskbar will show if any other applications are running. Close any that are shown there. If they are not closed it may be impossible for the installation program to install necessary files. Place the installation CD in the appropriate drive. The setup program on the CD will automatically start. If this does not happen, then run setup.exe on the CD.

The setup program will attempt to find any previous installation of the Essential Macleod. If it does then it will suggest that folder as the one in which the installation should be made otherwise it will suggest a default. Normally it will be sufficient just to confirm the choice of folder but it you do want the installation in a different folder or on a different drive then either use the browse button to search for the folder or simply type in its path, as, for example

C:\Program Files\The Essential Macleod

Note that you may enter any folder, not simply an existing one. If the folder does not already exist then it will be created. Should there be an existing installation that is to be upgraded by the current installation then one of the selectable options will be an upgrade rather than full installation.

Progress of the installation is now shown on screen with messages showing the names and folders of the files that are being installed. Some of these you will notice are going into the standard Windows folders. Along with all the program files, the setup program also creates a design folder with some demonstration designs and a materials folder with the standard materials supplied with the program. We have more to say about this below.

When the installation procedure is over then the Essential Macleod program can be found by clicking the **Start** button and selecting **Programs**. **Macleod** is an item in the programs list. Selection of the item reveals the program itself, recognizable by the admittance logo and the title **Essential Macleod**, an online manual called **Essential Macleod Manual** and a help file called **Essential Macleod Help.** To start the program itself, click **Essential Macleod**. Note that once the Essential Macleod is installed, it is not necessary to have Administrator privileges to run it.

Tools and Enhancements

The Essential Macleod contains a vast number of tools. A brief summary of these tools is shown below.

Core: Design Editors, Data, Target etc. editors, Import/Export, Materials management, Performance calculation, Refinement and synthesis, Export designs to various applications including Zemax, FRED, LinkSIM, VirtualLab and CODE V, Admittance loci, Electric fields, Design aids, Report generator

vStack: vStack editor, vStack performance calculation – calculate performance of non-parallel-sided substrates and coatings

Runsheet: Machine Configuration and Runsheet editor

Monitorlink: Special Runsheet configuration, Export monitoring programs, Free standing tool to link with specific controllers

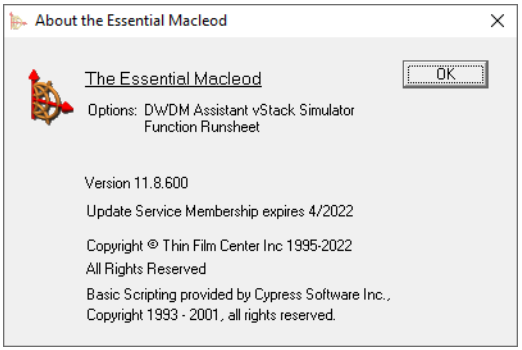
Function: Operation editor and syntax checker, Function evaluator

Simulator: Process deposition simulator

DWDM Assistant: Generates bandpass filter designs to meet a given specification

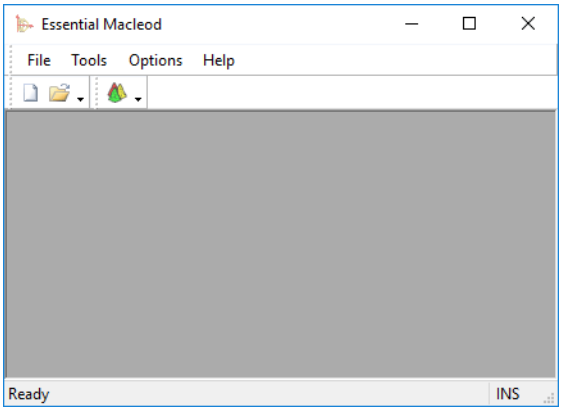
Which Tools Do I Have?

To find out which tools are present in any installation of the Essential Macleod, select the menu item **About the Essential Macleod** in the Help menu. An information box similar to the following illustration appears. Any enhancements that are present will be listed under the heading **Options** and will consist of any or all of **vStack**, **Runsheet, Monitorlink, Function** and **Simulator**. If none of these is shown then only the Core module is present.


About the Essential Macleod
The Essential Macleod
OK
Options: DWDM Assistant vStack Simulator
Function Runsheet
Version 11.8.600
Update Service Membership expires 4/2022
Copyright © Thin Film Center Inc 1995-2022
All Rights Reserved
Basic Scripting provided by Cypress Software Inc.,
Copyright 1993 - 2001, all rights reserved.

A QUICK TOUR OF THE PROGRAM

Double-click the Essential Macleod icon and the program will begin to load. The initial screen is quite blank with four menu items, **File, Tools, Options, Help**.

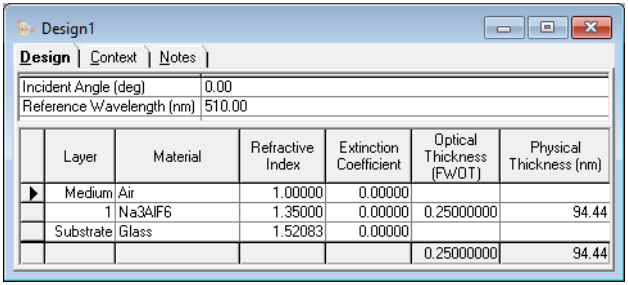


Select the **File** menu. It has several sections but the first carries the four principal items, **New, Open..., Open Material..., Open Substrate...** and **Open Function….**

Select **New**. The symbol, ▷ , at the end of the menu item shows that there is a submenu. The number of items depends on the configuration but there will be several, the first four being **Design, Material, Optical Constant** and **Table**.

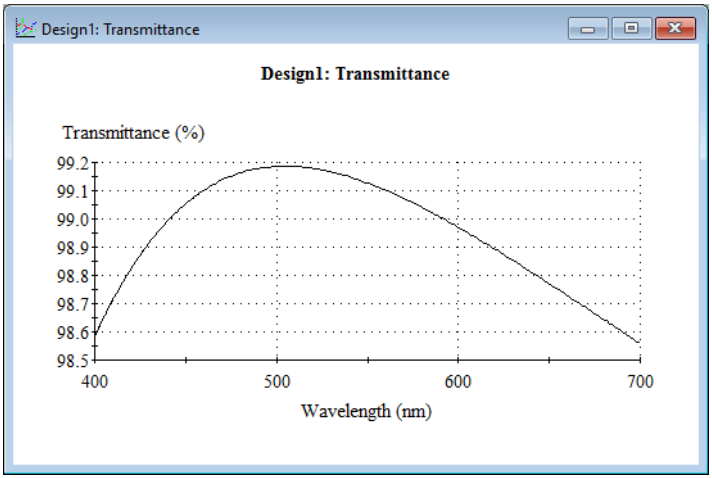
Select **Design** to open the Design window with a new design and a default design will appear. The idea of a default rather than a blank design is that all necessary parameters are initialized so that calculations can proceed without problems. The details of the default can be set by the user as described later in the manual but, if this is still the first time the package has been used the default will be a simple single layer coating.

Right at the top of the design window is the heading **Design1**. This is a default name that has been given to this design and, if not changed, will be the name of the design file in which the design will be stored. Next, immediately below the title, is the incident angle. This is the angle, measured in degrees, between the direction of the incident light and the normal to the coating surface. Here we have zero entered and so we are at normal incidence.



The reference wavelength is shown next. This is 510nm. In the initial configuration as the program is normally supplied, all wavelengths are given in nm. We will discuss wavelength units in detail later but for the moment we retain nm. The actual design is shown next along with the incident medium and substrate. The default convention used throughout the package is that the incident medium is uppermost in design tables. The substrate is the emergent medium and is at the foot. The layers are numbered in turn from incident medium to substrate so that the layer nearest to the incident medium is numbered one and is listed at the top of the table immediately after the incident medium. The other layers, if any, follow in order through to the substrate. The columns are labeled in turn, **Layer, Material, Refractive Index, Extinction Coefficient, Optical Thickness, Physical Thickness**. **Layer** lists the reference number of the layer or indicates the incident medium or substrate. The next three columns give information on the various materials, name and optical constants. Since we are dealing with dispersive materials the values of refractive index and extinction coefficient are those at the reference wavelength, λ_0, (which is 510nm currently). The optical thickness is next. This is nd/λ_0 where n is refractive index, d is physical thickness and λ_0 is the reference wavelength. 0.25, therefore indicates a quarterwave layer at the reference wavelength. [There are other options for the display of layer thickness and some other layer attributes (packing density, locked and linked) that are invisible for the moment, all of which we will consider later.] This design is therefore a quarterwave at 510nm of Na3AlF6 (cryolite) on glass in air and can be described as an antireflection coating. Let us examine the performance.

Select **Plot** from the Performance menu. A new window entitled **Design1: Transmittance** appears. The transmittance of the coating is shown plotted against wavelength from 400nm to 700nm.

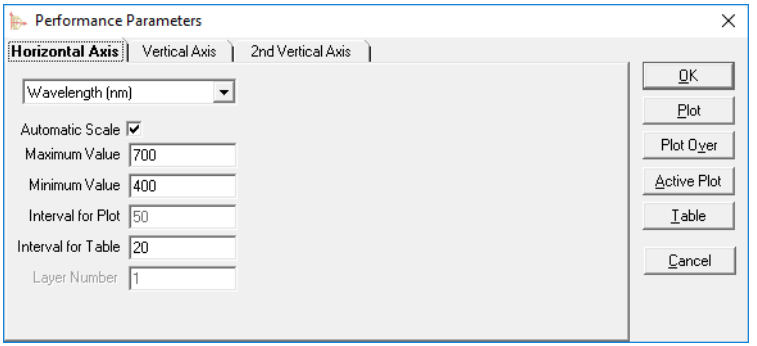


The transmittance is everywhere very high. Since this is an antireflection coating, reflectance may be a more suitable parameter to plot.

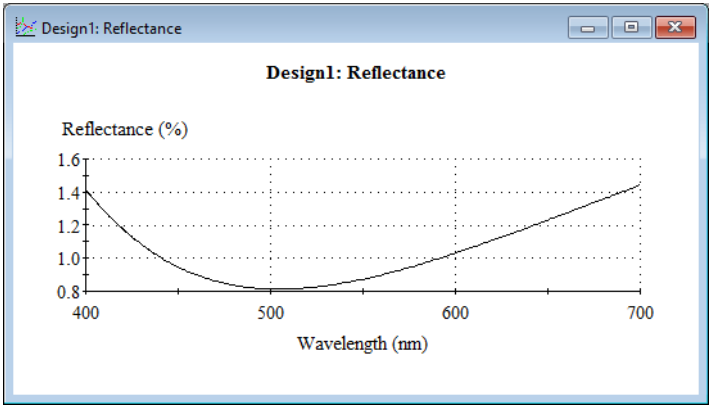
The active window is the plot, however, and so the current menu bar refers to it. We must therefore make the design window active so that the menu bar displays the design menu. To do this, place the mouse cursor over any visible part of the design window and click, or use the Windows menu. The design window should come to the front showing that it is active.

Before we change the plot, however, let us be sure that two plots may coexist. Select the **Options** menu and then **General...**The Essential Macleod Options dialog box will appear. Click the Windows tab. In this tab there is a check box labeled **Keep Old Plots and Tables Displayed**. Check this box if it is not already checked. Later you may wish to uncheck this box to automatically reduce clutter on your desktop.

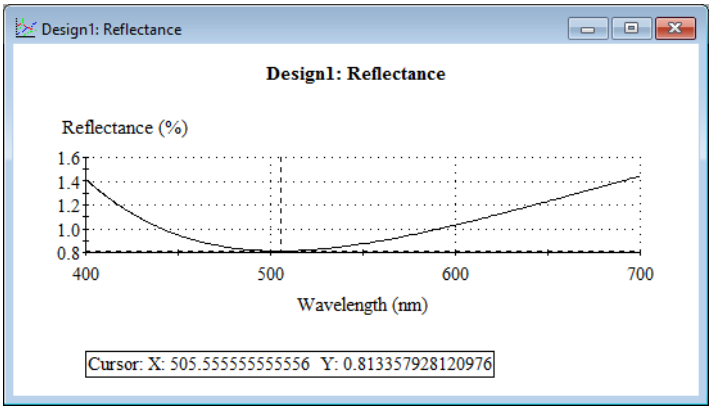
Now select the **Parameters** menu and the item **Performance...** The following dialog window opens. Note that some parameters apply only to certain choices of horizontal or vertical axis. Those that do not apply are shown in gray.



We want reflectance so we click the Vertical Axis tab and then set the performance to **Reflectance Magnitude (%)**. The vertical scale is listed as **Maximum Value 100**, **Minimum Value 0** and **Interval for Plot 20**. **Automatic Scale** is checked and so the plot will be re-scaled to fit the data. Leave all other parameters unchanged and click the **Plot** button.



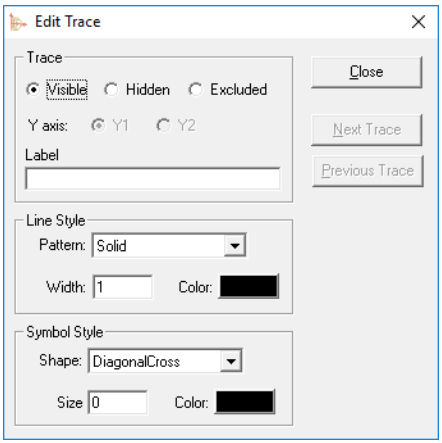
You can activate a cursor on the plot by holding down the **<Alt>** key and dragging the mouse over the plot with the left mouse button also pressed. A pair of markers will follow the curve nearest the mouse pointer and the (x,y) coordinates of the curve are displayed in a box beneath the plot.



The cursor is removed by selecting **Clear Cursor** in the Edit menu, or by right-clicking the mouse and selecting **Clear Cursor** from the menu that appears.

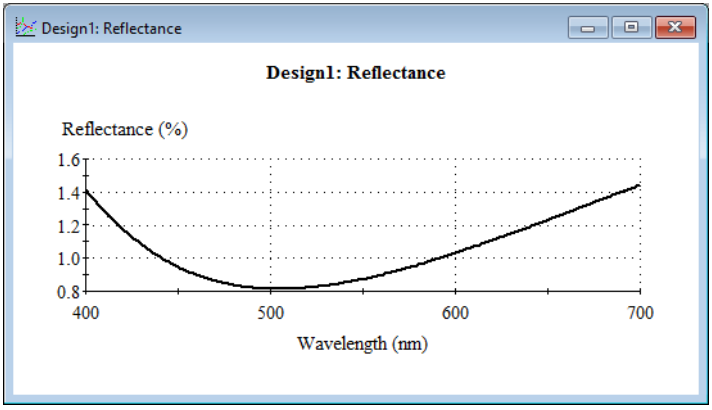
It is a good idea at this stage to remove any unwanted plot that has been generated so far. Click in a plot to make it active and then click the close box at the upper right corner. Do not accept the invitation to save the plot.

Now place the mouse over the performance curve and double-click. A new dialog box appears. This controls the display of the curve.



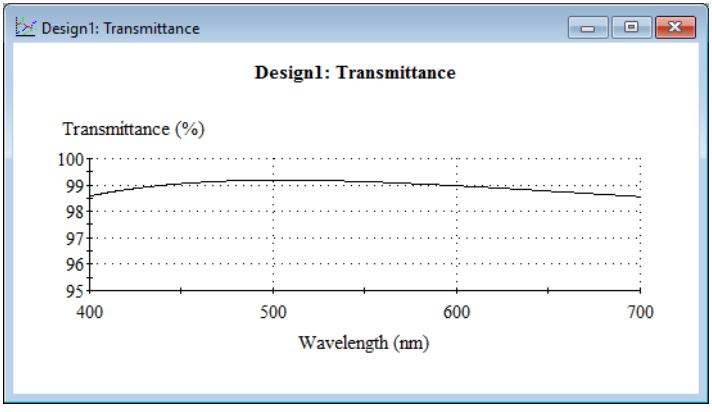
To change the thickness of the curve, enter a number into the **Width** box and click **Close**. This produces the plot below

It is important to realize, however, that editing the plot changes only the *parameters* of the plot. The data are unaffected. Thus the data cannot be changed from reflectance to transmittance just by altering the title of the vertical axis. Reflectance data remain reflectance whatever title is given to the axis.



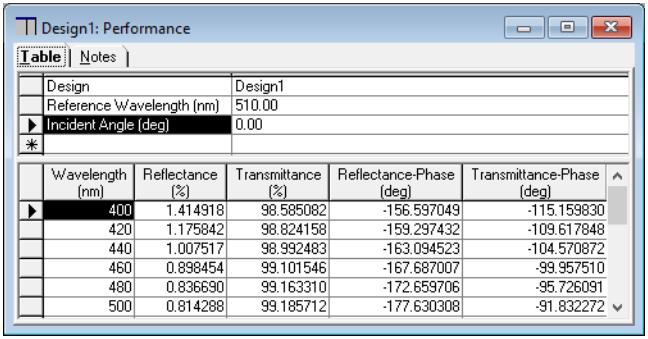
We will now save the plot. With the plot as the active window, select the **File** menu and then **Save As...** The **Save Plot As** dialog box appears. Note that there is a shortcut key, **F12**, that moves straight to the dialog box. Against **File name** type in **one**. Note that the extension for plot files will be **.npl** but that it is not necessary to add any extension. That will be done automatically by the package. Then select **Save**. The plot will be saved as file **one.npl**.

Choose **Performance...** from the **Parameters** menu. In the dialog box that appears select the **Vertical Axis** tab and then choose **Transmittance Magnitude (%)** with **Maximum Value** 100, **Minimum Value** 95 and **Interval for Plot** 1. Clear the **Automatic Scale** check box. Click the **Plot** button. The result is shown below.



Now examine the **Window** menu. It lists the various windows that have been created. Select each in turn and see how they come to the front. This is another way of making a window active and it is particularly useful when a window is completely obscured behind others.

Finally from the **Performance** menu select **Table**. The results are displayed in tabular form.



Design	Design1
Reference Wavelength (nm)	510.00
Incident Angle (deg)	0.00

Wavelength (nm)	Reflectance (%)	Transmittance (%)	Reflectance-Phase (deg)	Transmittance-Phase (deg)
400	1.414918	98.585082	-156.597049	-115.159830
420	1.175842	98.824158	-159.297432	-109.617848
440	1.007517	98.992483	-163.094523	-104.570872
460	0.898454	99.101546	-167.687007	-99.957510
480	0.836690	99.163310	-172.659706	-95.726091
500	0.814288	99.185712	-177.630308	-91.832272

Note that above the heading of the table are entries giving reference wavelength and incident angle. These entries are for reference only. It is possible to change these entries (the read-only status of the table must first be canceled) *but such changes will have no effect whatsoever on the actual values of the parameters, neither will they affect the values of the data in the table*.

The table lists values of reflectance, transmittance and phase changes on transmission and reflection at intervals that are determined by **Interval for Table** under **Horizontal Axis** in the **Performance Parameters** dialog box. The table window may have to be adjusted by stretching with the mouse in the normal way.

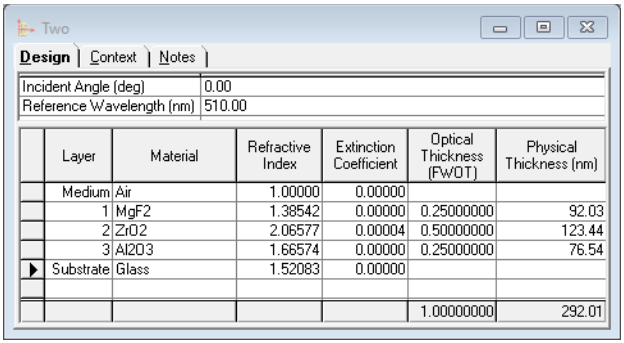
This current coating is not a particularly good one because the residual reflectance is too high for many applications. Also, although it has nothing to do with its optical properties, cryolite is not a rugged material. We will now examine a coating that is rather broader in its characteristic, and uses more resistant materials, but which is, at the same time, more complicated. This is the well-known quarter-half-quarter coating and the version we are going to examine consists of a quarterwave of magnesium fluoride outermost followed by a halfwave of zirconia, and then next to the substrate a quarterwave of alumina. The pattern of this coating is a low index quarterwave next to the incident medium and an intermediate index quarterwave next to the substrate which form an antireflection coating for the reference wavelength. These layers are separated by a flattening halfwave of high index, which gives added breadth to the characteristic. The names for the materials in the materials list are mostly based on the chemical formulae and the materials we are suggesting have names MgF2, ZrO2 and Al2O3 respectively.

Save the design in a file named **one**. The name at the top of the design window will change to **one**. We want to keep this design. It is, however, still the active one. Any changes we make now will risk being incorporated in **one.dds** should an automatic save be initiated. To avoid this we immediately save the design yet again as **two.dds**. Press **F12** and enter **TWO** (or **two**) in the **File Name** box and then select **Save**.

This is really good practice that is worth cultivating. It is all too easy to lose a design by overwriting it. It is usually impossible to recover a design once it has been overwritten although the Undo and Redo commands (in the Essential but not the Concise) may come to the rescue. This procedure is particularly useful also when many of the parameters remain unchanged. When you want to start a completely new design, use the **New** command in the **File** menu. The new design will then coexist with the previous one, which will not be automatically closed. Being able to edit several designs at the same time is a valuable feature of the Multiple Document Interface (MDI) of the program.

We will now edit the design **two.dds.**

There is only one layer in the current design and we need three. The first task is to increase the number of layers to three. Place the cursor over a cell in the row corresponding to the cryolite layer (Na3AlF6, Layer 1) and click. Now go to the **Edit** menu and select **Insert Layers...** In the resulting dialog box enter **2** as the number of layers to be inserted and then select the **OK** button. Now the design will show three similar layers of Na3AlF6. The material for layer 1, that next to the incident medium should be magnesium fluoride, MgF2 in the materials list. Place the cursor over the cell in layer 1 containing Na3AlF6 and click. The cell will be selected and a small arrow will appear at the right. A click on the arrow brings up a small scroll box with the names of the existing materials in it. MgF2 is a little way down the list. Click on it and immediately the name of the material for layer 1 will change to MgF2 and the scroll box will close. The insertion of the extra layers resulted in a thickness of zero for layer 1. This must be changed to the required 0.25. Place the cursor over the thickness cell for layer 1. Click once to select it. Then type **0.25**. Note that as soon as we selected the thickness cell, deselecting the material, the value of refractive index changed to match the index of magnesium fluoride at the reference wavelength. Incidentally, a double-click in the thickness cell will place it in insert mode and then anything typed will be added to what is already there. If that happens then use the Delete key to remove the unwanted characters. Now we pass to layer 2. Here we need a halfwave of zirconia, ZrO2. The same process as before permits us to replace the Na3AlF6 material with ZrO2. The zero thickness must then be changed to **0.5**. Finally we change the material for layer 3 to Al2O3. This time, instead of selecting the layers from the list, select the materials cell and type in **Al2O3**. Now select any other cell. The entered material will change to Al2O3 denoting that the new material has been accepted by the program and the **Refractive Index** cell will display the appropriate value at the reference wavelength. Materials can be entered either manually or from the table. Sometimes manual entry can be quicker than looking up the table each time. The thickness of layer 3 is already 0.25 (if the insertion was performed exactly as described here) and so it needs no alteration. At this stage the design window should appear as reproduced below:

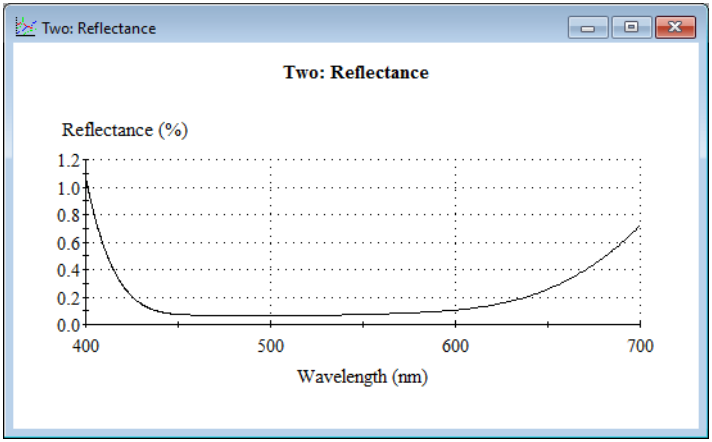


Incident Angle (deg)	0.00
Reference Wavelength (nm)	510.00

	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
	Medium	Air	1.00000	0.00000		
	1	MgF2	1.38542	0.00000	0.25000000	92.03
	2	ZrO2	2.06577	0.00004	0.50000000	123.44
	3	Al2O3	1.66574	0.00000	0.25000000	76.54
▶	Substrate	Glass	1.52083	0.00000		
					1.00000000	292.01

We added the layers by using the insert layers command. There are several other ways of performing this task and a particularly useful one is available when the **INS** (insert) mode is visible in the bar at the foot of the Essential Macleod window. (If **OVR** is shown then press the **<Insert>** key and the mode will change to **INS**.) Place the cursor in a cell on one of the layers. Press **<Enter>** repeatedly, each time making the cell to the right of the current one active. When the thickness cell is active, pressing **<Enter>** will create a new layer. A layer that is unwanted can be deleted very quickly by clicking in the little square selection box at the extreme left of the layer and then pressing **<Delete>.** This method of adding and deleting layers is very useful when a number of layers is being entered by hand.

Now we plot the performance of this new design. In the parameters dialog, set the vertical axis to be Reflectance Magnitude and check the Automatic Scale box. Now click Plot



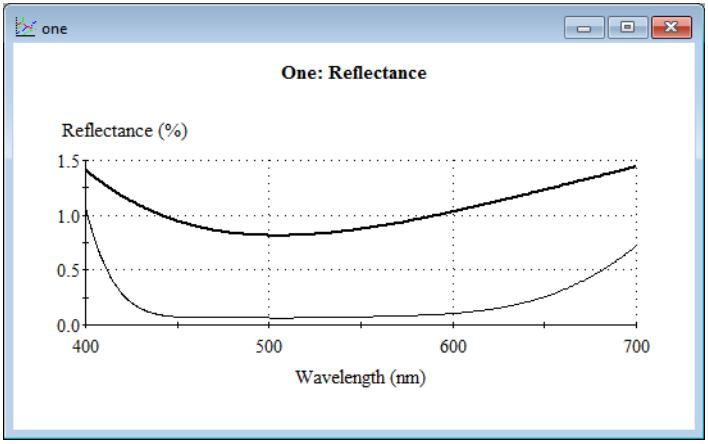
Save this plot as plot file **two** using the same procedure as before, that is selecting the plot by making the plot window active and then using the **Save As...** command in the **File** menu, or, pressing **<F12>**.

It would be useful to compare these two plots in the same diagram. To illustrate how this can be done let us close all the plot and design windows. Now either go to the **File** menu and select **Open...**, or press **<Ctrl><F12>**. This brings up a dialog box with a list of files to open.

A list of design files is shown but we want the plot files. Click the arrow to the right of the **Files of Type:** window and select **Plots**. The list of designs will disappear to be replaced by the list of plots that we have saved so far. Select **one.npl**. This is the plot corresponding to the single layer. The line thickness was made perhaps rather too large . Let us change that to a fine dotted line. With the mouse over the curve, double-click the left mouse button. In the dialog box that appears change the Pattern to be **Dotted** and then click **Close**. This changes the appearance of the curve.

Now we want to add the three layer antireflection coating curve to the same diagram. Return to the **File** menu and select **Add Line...** This time there is no equivalent single key stroke but you can use **<Alt><F>** followed by **<d>**. The **Add** dialog box appears and this time the file **two.npl** can be selected. Both curves are now on the same diagram as shown below. This plot may in turn be stored for later recall or for adding further curves.

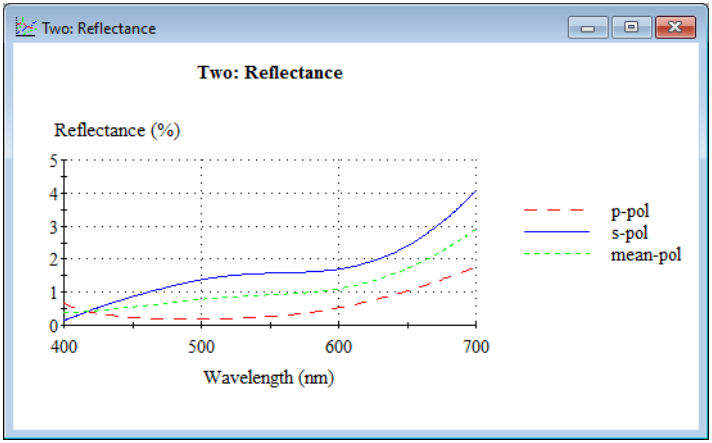
An alternative way of combining plots is to drag one plot over another. Of course the plots should be compatible, especially the horizontal axis.



It would be interesting to see how the three-layer coating operates at oblique incidence. Open the design named **two**. Let us choose an angle of 45°. This can readily be entered in the cell labeled **Incident Angle** right at the top of the **Design** window (or in the **Performance Parameters** dialog box). We decide we want to plot both s- and p-polarizations together with the mean. We therefore select the **Parameters** menu and **Performance...** Down at the foot of the resulting dialog box there is a set of polarization check boxes. Check **P**, **S** and **Mean**. Select **Plot** either by clicking the plot button or selecting **Plot** from the **Performance** menu and the result is as shown below.

In the normal configuration of the package, the curves will all be full lines but with different colors, red for p-polarization, blue for s-polarization and green for mean. In this version of the plot the s-polarization curve is the full line, the p-polarization the broken

line with broad dashes and the mean the broken line with short dashes. This is so that it can be printed in black and white if necessary.



A Word about Data Files

The program generates many different files containing data as it operates. You will want to preserve various designs that have been entered. Significant plots and tables will be stored. Specifications for refinement will be created. Text files with pasted-in design and performance details for incorporation in reports will be saved. The amount of material that can accumulate in one project is enormous and from time to time you will want to archive this data and start again. If all of this is preserved in a dedicated folder, then archiving and clearing out is straightforward. If, however, it is mixed in with program files and with other project files then there can be a real problem during archiving. The program is arranged so that many different design folders can be used. These must first be created in the usual way (Windows Explorer is simplest). Try to adopt a convention in naming the folders so that they have a clear and obvious meaning. This will help enormously in keeping things organized. The Jobs facility (see the section Work Data Management if the chapter The Essential Macleod Structure for more information) can be of great help in this.

...about Materials Databases

Many materials databases can be used. The only limitation is that only one database at a time may be active. The databases are completely separate entities and can contain duplicate names without any risk of ambiguity because the design files are linked to the materials database with which they were created. Thus a separate database with subtle differences in material properties could be maintained for each coating plant. Two databases, one labeled WET and the other DRY could permit rapid calculation of the effect of moisture on different filters. Although the coating design files are linked to their own materials databases, nevertheless it is very easy to change from one database to another with the same material names. It is simply difficult to do it accidentally.

It is also possible to vary variable units from one database to another. Coatings for the far infrared are better handled in microns that in nanometres, for example.

A materials database is a collection of material files that are held in a separate folder together with control files. The collection can be as extensive or narrow as desired. The easiest way to create a material database is to type the name including path in the **Materials Folder** window in the **Essential Macleod Options** dialog box. Choose **General...** in the **Options** menu to activate the dialog box. If the name that has been entered is a new one then the program will automatically create the new database. Another way of creating a materials database is simply to copy an existing one into a new folder. It is most important that the control files should be kept in the same folder as the material files otherwise the material files cannot be used by the program. Rather like the design file folders, the names of materials databases are best chosen carefully so that they convey an idea of their content. IR, VIS and UV, for example convey immediately the idea of spectral regions and differences in wavelength units. PlantA, PlantB or ClientA, ClientB are also designations that convey an immediate meaning. Note that a separate materials database is automatically created as part of any new job.

...and about Conventions

There are conventions concerning designs and parameters that are dealt with in detail in the next section but some are so important that we mention them also here.

The term, **Medium**, refers to the incident medium and **Substrate** to the emergent medium. In the default convention, designs are written with the flow of light from left to right or from top to bottom so that a formula representing a design is assumed to have the incident medium on the left and the substrate, or emergent medium, on the right. The designs shown in the design window have incident medium at the top of the table and emergent medium, or substrate, at the foot. This default convention can be changed. See the Options Menu section in the chapter APPLICATION WINDOW. [Note that throughout the Macleod packages there is just one exception to this rule and that is in Runsheet where the order of the layers is necessarily that in which they are deposited, that is with the layer next to the substrate first - although there is provision for accommodating a coating where the incident medium might be a prism with a coating on its hypotenuse.]

Layer thicknesses may be specified in four principal ways. Optical thickness is given by nd/λ_0 or by $4nd/\lambda_0$ (QWOT), geometric by d/λ_0 and physical by d where λ_0 is the reference wavelength, n, the real part of refractive index, and d, the physical thickness of the film, that is the thickness that would be measured by a conventional ruler.

There is a hierarchy that determines the way in which thicknesses in a design change when the reference wavelength is changed. If optical thicknesses are displayed, then they remain constant when the reference wavelength is altered. This implies that the physical thicknesses will change. If, however, optical thicknesses are missing, but physical thicknesses are displayed, then the physical thicknesses will remain constant. Geometrical thicknesses will remain constant only if the other two conventions are missing. The item **Display Setup** in the **File** menu governs what is displayed.

However, when layers are copied and pasted, it is the physical thickness that remains constant in that operation because it is assumed that the properties of the pasted layer should be exactly those of that copied.

CONVENTIONS

Conventions are important because they define the frame of reference used for the results and when comparing results from two different sources they become vital. We therefore discuss in this section the primary conventions that are used in this package. Note that these conventions are applied uniformly throughout the Essential Macleod and package so that results obtained in any section are completely compatible with those obtained in any different section. If, therefore, you will be confining yourself to use of the Essential Macleod and no other thin film packages then you may wish to omit this somewhat tedious section on, at least, a first reading. It is here should you ever need it. [If you are going to be involved in the calculation of relative phase shifts between s- and p-polarized light then it could be useful to skim through the part dealing with the convention for the calculation of Δ.]

The term, **Medium** refers to the incident medium and **Substrate** to the emergent medium. This terminology is the usual one in thin-film coating design. The default convention is that the medium is at the top of a design and the substrate at the foot. Then the layers are numbered from 1 at the outer surface next to the incident medium to the total number of layers at the substrate (i.e. emergent medium) interface. This default convention is followed throughout the package with one exception - Runsheet. The convention in Runsheet is that the layer next to the substrate is always layer number 1. Note that the conversion from the default layer numbering convention to the Runsheet layer numbering convention is automatic, you do not, and indeed, must not alter the design before loading it into Runsheet.

Not everyone prefers this default convention. It can be changed in the General item in the Options Menu. More details are in the Options Menu section of the APPLICATION WINDOW Chapter.

Designs, in the default convention, are written with the flow of light from left to right or from top to bottom. A formula representing a design is assumed to have the incident medium on the left and the substrate, or emergent medium, on the right. This, too, can be changed as explained in the Options Menu section.

Layer thicknesses may be specified in four ways. Thicknesses may be either full-wave optical thickness (FWOT) or quarter-wave optical thickness (QWOT) or geometrical or physical. Physical thickness is just the thickness of the film as it would be measured by a ruler calibrated in physical thickness units, nanometres unless they have been changed by the user. In interference calculations the most important quantity associated with a layer is its effect on the optical phase of light that traverses it. The phase change depends on the optical path and the vacuum wavelength. Full-wave Optical thickness, therefore, is the physical thickness multiplied by the refractive index of the material (that is the optical path) and divided by the reference wavelength. Because of its fundamental role in calculations, it is frequently used in preference to the other thickness conventions. QWOT thickness is another type of optical thickness. 1 QWOT is equal to 0.25 optical thickness units. Geometrical thickness is the ratio of physical thickness to reference wavelength.

One of the reasons we often use the ratio of the thickness of a layer to a reference wavelength is that dimensionless quantities are usually to be preferred over dimensioned

ones with units. Many of the layers in the designs considered so far have optical thicknesses (FWOT) of 0.25. This means that the optical path for one traversal is one quarter of a vacuum reference wavelength. The material for one layer, listed as Na3AlF6,is cryolite or Na_3AlF_6, and the refractive index of this material is shown as 1.35. This is the value at the reference wavelength which is 510nm in this case. We can tell that the geometrical thickness would be 0.25/1.35 that is 0.185185. Physical thickness would be 94.444nm.

The reference wavelength, λ_0, is simply, as the name suggests, a reference value of wavelength to which parameters such as optical thickness are referred. It is usually chosen as a meaningful wavelength, that at which the layers are quarterwaves, for example. As far as changing the value of the reference wavelength is concerned, we can do this at any time by activating the design window, selecting the Reference Wavelength cell by clicking within it and typing in the new value.

Layer numbering can be set in the Design tab of the General Options window to run either from the substrate or from the incident medium. In Runsheets, the displayed order is always in deposition order and so there the top layer, numbered 1, is the one next to the substrate.

The aspects of performance that are principally addressed in the Essential Macleod are connected with the specular reflection, transmission and absorption of light. The system that is assumed in all of the calculations is a smooth, flat surface of a substrate, or emergent medium, over which has been applied a layer or series of layers of different material such that the interfaces are smooth and parallel both to each other and to the surface of the substrate. The materials are generally isotropic but may be biaxially birefringent and, in much of the package, homogeneous. (These are all quite normal constraints). There is an incident medium in which a collimated beam of monochromatic light is directed at the coated substrate. The incident medium must be isotropic. The light is partially reflected, transmitted and absorbed by the system. The layers are considered to support interference and so the calculations involve all the interfering beams that are reflected backwards and forwards within the layer system.

The materials are characterized by their optical constants n and k. There are two physical aspects of the optical constants, refractive index and optical admittance. These quantities are numerically equal at optical frequencies but physically different. Refractive index is the ratio of the velocity of light in free space to that in the medium and is purely a property of an optical material while optical admittance is the ratio of the magnetic field amplitude to the electric field amplitude. Optical admittance may be either an attribute of a material when it is known as the characteristic optical admittance and is the ratio of the amplitudes of a progressive harmonic wave, or an attribute of a thin film structure when it is known as the admittance of the structure and is the ratio of the total fields of the interfering waves. Refractive index is a pure number and may be written as (n-ik) while the characteristic optical admittance is (n-ik) free space units. [A free space unit is 1/377 siemens] There is a convention involved in the minus sign before the ik. In some publications a plus sign may be shown and this is an indication of the opposite convention for the progressive wave considered below. The terminology for n and k is somewhat unfortunate because n is usually called refractive index while k is known as the extinction coefficient. When it is necessary to differentiate between n and (n-ik), the former is referred to as refractive index or sometimes real part of refractive index while

the latter is the complex refractive index. In the package refractive index is used to refer to n and extinction coefficient to k. The package handles all conversions into complex numbers and optical admittances automatically and discretely. The extinction coefficient, k, is an indicator of any absorption in the material. When it is zero the material is completely free from absorption. Dielectric materials have small or zero values of k, while metals have very large values.

Where materials are biaxially birefringent., three sets of optical constants are required. The principal axes of the birefringent material are parallel or perpendicular to the surfaces and to the principal plane. In the material editor these axes are labeled x, y and z. The x-axis and y-axis will be in the plane of the films. The *z*-axis will be normal to the film plane and into the system in the direction of the incident light. We associate the x-axis with *p*-polarization and the *y*-axis with *s*-polarization. The direction of incidence will be in the x-z plane rotated in the incident medium through ϑ_0 about the positive y-axis.

The system is assumed to be completely linear in its response and so the performance may be described in terms of dimensionless quantities that are normalized with respect to the appropriate attribute of the incident light. Reflectance is the ratio of the reflected irradiance to the incident irradiance. (Irradiance is the mean power per unit area transported by the wave. In the SI system of units it is measured in watts per square metre [Wm^{-2}]. An older term for irradiance is Intensity). Transmittance is the ratio of transmitted irradiance to incident irradiance. For these ratios to be meaningful, the incident medium must be free from absorption. This is not a serious limitation because it is impossible to make a measurement of reflectance in a medium that has even slight absorption. The program will not accept an extinction coefficient other than zero for the incident medium, any non-zero extinction coefficient in the material file for the incident medium is ignored. [We emphasize that this is not an inherent limitation of the program but a well-founded result in fundamental optics. Incident and reflected irradiances can no longer be separated because of a varying coupling between them. If they cannot be separately measured then reflectance cannot be defined.] In interference calculations especially, and also in many other applications, changes in the amplitude of the light are important. Light is electromagnetic and so there are strictly two amplitudes associated with it, the magnetic field amplitude and the electric field amplitude. At optical frequencies direct magnetic effects may be neglected and any interaction with matter is overwhelmingly associated with the electric field. The accepted convention, therefore, is that the word amplitude, with no qualifier, is always taken to indicate the electric field amplitude. Both the magnitude and the phase of the amplitude are equally important. The magnitude can readily be derived from reflectance and transmittance data, so the primary performance is usually left in terms of reflectance and/or transmittance. The phase of the light must be calculated separately, but to do this unambiguously we need to define the form to be used for the progressive wave. As is usual this is written in the complex form and we adopt the normal convention in thin film optics for a progressive wave in the *z*-direction as

$$E = \mathcal{E} \exp i \left[\omega t - \frac{2\pi(n - ik)z}{\lambda} + \varphi \right]$$

which can be written

$$E = \left\{ \mathcal{E} \exp\left[-\frac{2\pi k z}{\lambda} \right] \exp[i\varphi] \right\} \exp\left[\omega t - \frac{2\pi n z}{\lambda} \right]$$

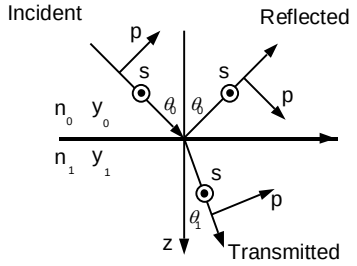
where our minus sign in the complex refractive index is seen to be necessary for the wave amplitude to exhibit a decrease with propagation distance in an absorbing medium. The part of the wave expression in the curly brackets is known as the complex amplitude and it includes the *relative phase*. The final exponential is known as the *phase factor* of the wave. When the superposition inherent in interference calculations is concerned it is usual to arrange that the phase factors for all waves are exactly in that form so that they can be eliminated from the calculation that then proceeds in terms of the complex amplitudes only.

Phase change on reflection is the change in phase φ that is suffered by the light on reflection. There is a problem in that the reflected beam is propagating in the opposite direction so that the phase factor has the form

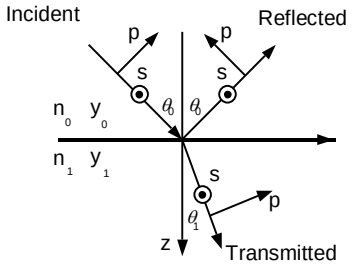
$$\exp i\left[\omega t + \frac{2\pi n z}{\lambda} \right]$$

and does not cancel with the phase factor of the incident wave. The phase difference between the waves is a function of *z*. The convention used virtually universally is to define the origin of the *z*-axis as the interface where the reflection is taking place, normally the front interface of the multilayer. Then *z* is zero in both waves and the phase factors are then equal and can be eliminated. *Reflected phase shift*, therefore, is by convention the *difference in phase measured exactly at the point where the reflection is taking place*. Throughout the package this point of reference is the front surface of any thin film system, that is the interface with the incident medium. This is particularly important in the calculation of the influence of uniformity on wavefront, for example.

There is less of a problem in transmitted phase and no clear consensus on a definition. The phase factors have the same form and can be made exactly equal by including any relative shift in *z* in the phase difference. In this package the phase change is calculated as between the emergent beam at the point it enters the emergent medium or substrate and the incident beam where it enters the coating and leaves the incident medium. This means that it includes a phase change corresponding to a displacement along the z-axis equal to the total thickness of the coating. Again this is important if calculations of the consequences of coating uniformity on a wavefront are being performed.



The normal thin film convention for electric field directions in reflection and transmission. This convention is used in the package for all calculations with the sole exception of Δ in reflection.



The convention for electric field directions for calculations of Δ in reflection and for all calculations including Δ in transmission.

At oblique incidence the performance depends on the state of polarization of the incident light. There are two eigenmodes of polarization called s-polarization (electric field normal to the plane of incidence) and p-polarization (electric field parallel to the plane of incidence). [An eigenmode of polarization is simply a mode where the state of polarization is not changed in either reflection or transmission and so any general case can be expressed as a combination of given proportions of the eigenmodes which can then be computed separately.] There is often interest in the difference in phase between the p-polarized and s-polarized components of a beam. This is given the term *delta* or Δ. Δ is nominally given by $\Delta = (\varphi_p - \varphi_s)$ but there is a slight complication. The normal convention for phase shifts on reflection in thin film calculations is that shown in the first of the two preceding figures. The normal convention for the calculation of Δ, however, reverses the direction of the electric field in the p-polarized reflected beam. Calculations of the phase difference between s- and p-polarized light on reflection therefore follow the normal convention in the first figure while the calculation of Δ follows the convention in the lower figure. This involves a difference of 180° or π in the value of Δ compared with $(\varphi_p - \varphi_s)$.

The angle of incidence is always referred to the incident medium throughout the package. [In the Stack editor the substrate for one coating may be the incident medium for another but the overall angle of incidence for the entire structure is likewise in the incident medium.] This incident medium is a dielectric because of the theoretical limitations mentioned above. This implies that the incident wave in all calculations is always homogeneous although the waves in absorbing films or substrates will be inhomogeneous (planes of constant phase and planes of constant amplitude are not coincident). The user need not be aware of this complication which is handled completely automatically by the package.

THE ESSENTIAL MACLEOD STRUCTURE

The Core of the Essential Macleod is an integrated set of tools for carrying out the operations involved in the design and analysis of optical coatings. In this there are five main tasks.

1 The calculation of the performance of a given design
2 The derivation of a coating design given a desired performance
3 The maintenance of optical constant data for the materials
4 The analysis of the design for improving understanding
5 The incorporation of the design as a component of a complete filter

Adding tool groups known as Enhancements further extends the capabilities of the Essential Macleod. There are currently five such groups, Function, Runsheet, Simulator, vStack and DWDM Assistant. These are the subjects of later sections of the manual. Briefly, Function is concerned with extending the range of capabilities by enabling a wide range of additional operations on data produced by the core tools. Runsheet is concerned with the conversion of design data into production control programs. Simulator is concerned with modeling the production of optical coatings. vStack calculates the performance of systems of coatings that are not parallel but have coplanar normals. DWDM Assistant designs narrowband filters primarily for telecom applications and made up entirely of quarterwaves and exact multiples of quarterwaves. An additional tool, Monitorlink, that communicates with one supported controller is supplied on request.

Performance Calculation

Reflectance, transmittance, phase change on reflection, phase change on transmission, absorptance, density, the ellipsometric parameters ψ and Δ in reflection and transmission, their derivatives up to third order with respect to λ, the ultrafast parameters, group delay (GD) group delay dispersion (GDD) and third order dispersion (TOD), and color coordinates are the major parameters calculated in the Essential Macleod. These can be examined over a range of wavelengths, frequencies and angles of incidence and also thickness variation of a chosen layer all with completely flexible units for the independent variables. The results can be presented in the form of tables or of plots that can be stored for later recall and manipulation or can be cut and pasted into other applications.

The effects of layer thickness errors can also be calculated so tolerance estimates may be made.

The designs may be exported to the Zemax lens design package produced by Zemax LLC, to the Code V lens design package produced by Optical Research Associates, to the FRED optical modeling package produced by Photon Engineering, or to a filter file for LinkSIM produced by Rsoft Design Group Inc.

Thermal Model

The Essential Macleod provides a model for estimating the effects of temperature variation on the optical performance of a coating that is based on the model that was developed by Haruo Takahashi (H. Takashashi, “Temperature stability of thin-film narrow-bandpass filters produced by ion-assisted deposition”, Applied Optics, Vol 34, No. 4, Feb 1995 pp667-675). The model assumes linear behavior of single-phase material. Strain-induced changes in refractive index are assumed to be isotropic through a packing density mechanism. The important parameters of the model are the linear expansion coefficient, the temperature coefficient of refractive index and Poisson’s ratio. These parameters may be specified for each material with the Material editor. Changes in layer properties are assumed sufficiently small so that second-order effects may be neglected. Interdependence of any of the important film parameters is also neglected.

A temperature is entered as an offset from an unspecified reference temperature. At the reference temperature, materials have the optical properties defined in the materials tables and zero strain is assumed in all layers and the substrate. For non-zero temperature offsets, strain is introduced into the layers by the differential expansion of the substrate and the layers. This causes the thickness of each of the layers to change and also the packing density. The refractive index of each of the layers also changes due to the temperature coefficient of the refractive index of the material.

The thermal model is implemented in the Design editor and in Simulator. In the Design editor, performance can be calculated for a specified temperature offset.

Simulator models the effect of changing temperatures during manufacture. A temperature profile defines how the temperature changes during deposition. At the start of deposition of a layer, the substrate and layers already deposited are raised to the deposition temperature of the layer. The layer is then deposited at the temperature offset. Layer thickness is determined by the monitoring method used taking into account the changes to the optical properties of the coating caused by the temperature offset. Once deposition of the layer has completed, the substrate and layers are returned to the reference temperature in preparation for the next layer.

When you use non-zero temperature offsets, you will be warned if thermal data is missing from any of the materials.

Uniformity Model

A coating machine will typically show a variation in deposited thickness across the area where parts may be coated. The magnitude and form of the variation depends upon the construction of the coating machine. The variation depends upon the location and form of the material sources and so the magnitude and variation will typically be different for each material source. In the coating machine (when properly calibrated and neglecting production errors) there will a location where the manufactured part will have the designed thicknesses. We will call this the Reference Location. Parts at some distance from this reference location will have thicknesses that are not the designed thicknesses caused by the non-uniformity of the coating machine. Some layers may be thicker than the design thickness and some other layers may be thinner. This will cause changes in the performance of the design. The Essential Macleod provides a simple one-dimensional linear model of uniformity that allows the impact of non-uniformity to be investigated.

Each material has a Taper Factor parameter. In uniformity calculations, a Taper Distance is specified. During the performance calculation, the thicknesses of the design are modified as follows:

NewThickness = (1 + Taper Distance * Taper Factor) * Layer Thickness

Where Taper Distance is in arbitrary units.

Taper Distance may have negative as well as positive values. Taper Factor may also be positive or negative. Uniformity calculations are available in 3D plots (choose Taper Distance for the x or y parameter) and in Active Plots for Designs (add the Taper Distance variable).

Coherence, Cone and Bandwidth

Coherence is a system parameter expressing the strength of interference effects. Interference effects can be reduced by variations in parameters such as wavelength, angle of incidence, thickness, and so on. When interference effects are completely undiminished we describe the process as coherent, or, sometimes, as exhibiting complete coherence. When interference is completely suppressed we use the term incoherence. Intermediate processes where interference fringes are reduced, but not eliminated, are described by the term partial coherence. In the Essential Macleod the two principal conditions are complete coherence or incoherence. We assume in normal calculations that films in a design exhibit complete coherence, that is interference effects are completely undiminished. We likewise assume that elements that we call media, and are thick slices of material described as parallel or wedged, exhibit complete incoherence, that is where no fringes are present. In incoherent calculations, multiple beam summations involve addition of irradiances with no attention paid to relative phase. These selections are automatic and are usual in optical coating calculations.

What of partial coherence? Here we have two tools that help us, Cone and Bandwidth. These tools appear whenever a parallel or wedged medium is declared in a Design document or whenever we use a Stack document. They are available in the vertical axis parameters.

Bandwidth assumes a rectangular response function with a constant width in units of wavelength. Digital calculation of the response cannot be continuous but must involve a wavelength step that can be set in the Cone tab of the General Options dialog. However, whatever the setting there will always be a minimum number of steps in the calculation. Note that when the fringes are completely regular, as from a single thick film or foil, there may be a type of beating visible in the response. This is a natural interaction between a scanning function with width constant in wavelength and a scanned repeated feature with width constant in frequency.

The cone can be Lambertian, when it is expressed in terms of semi angle, focal ratio or numerical aperture, or it can be Gaussian when it is expressed in terms of beam divergence or beam waist. It is also possible to specify through a text file the variation of power density in the cone.

A Lambertian cone mimics illumination from a Lambertian radiator, that is one that has the same radiance at any angle. Black bodies, for example, are Lambertian radiators. The illumination is defined as Lambertian within the cone but zero outside it. However the surface of the coating is specular, not Lambertian, and so there is a cosine effect at the

illuminated surface of the coating and this is taken into account in the calculation. The Lambertian cone includes the effects of polarization that must be unambiguously defined. We imagine a plate polarizer inserted in the cone and normal to its axis. The polarizer permits passage only of that light that has its electric vector is in the permitted direction. The permitted direction is everywhere parallel in the polarizer. When that direction is aligned parallel to the principal plane of incidence, defined by the cone axis and the surface normal, the polarization is defined as *p*-polarization. When the permitted direction is normal to the principal plane, the polarization is defined as *s*-polarization. Calculated mean polarization in this particular case is actually unpolarized light, but the term mean is retained for consistency. Under some circumstances unpolarized results can differ very slightly from the mean of *s* and *p*-polarizations. The Lambertian cone mimics the illumination occurring in many optical instruments where there is a light source and a condensing system.

A Gaussian cone is similar to a Lambertian cone in terms of the way its polarization is defined but the irradiance in the cone falls off from the cone axis as a Gaussian function and there is a phase correspondence amongst the various rays in the cone. The cone apex semi angle (Gaussian Semi Angle in the Essential Macleod) then defines the asymptotes of the cone, which are defined as the angle where the irradiance has dropped to $1/e^2$ of its axial value. Because of the phase correspondence, the cone converges to a Gaussian spot and then expands. The spot diameter, still defined by the asymptotes, is known as the beam waist, or in the Essential Macleod Performance Parameters dialog, as the Gaussian Spot. The Gaussian Spot is inversely proportional to the apex angle of the Gaussian cone and so the two are not independent. There is strictly no actual limit to the Gaussian function but the irradiance does decay rapidly outside the asymptotes of the cone. However the lack of a definite limit makes calculations at large angles of incidence coupled with large apex angles, exceeding 90° in total, problematic and they should be avoided. The Gaussian cone calculations are intended to mimic the illumination from a laser or the effects of a small illuminated spot.

Then there is the ability to model a cone with arbitrary illuminating distribution of power density. The source can be considered to be a sphere at a large distance and centered at the coating and emitting unpolarized light. The power density of the illumination from the sphere is defined as a function of the angle measured from the cone axis, the axis being at zero angle, but there is no variation with azimuth angle. This calculation option is indicated by Profile in the list of cone options in the Performance Parameters dialog. The power density distribution is defined in a reference file that lists power density against angle. The angle need not be defined at constant interval and the power density value will be extrapolated as constant at either end (the normal extrapolation method in the Essential Macleod). If a truncated set of angles is to be used with no input outside the angular range, then the terminating values must be set to zero. The extrapolation will use the terminating values. The cone shares its definitions of polarization with the Lambertian and Gaussian versions and can be tilted to any angle of incidence. As an example, a reference file with two entries, 20° with 1.00 relative power density, and 70° with 1.00 relative power density, and set at zero angle of incidence, will yield an answer indistinguishable from a Lambertian Cone with zero incidence and 90° Semi Angle. We can truncate the range to be calculated by inserting 19.999° with zero power density before the 20° entry and 70.001° with power density zero after the 70° entry. It is important to note that the power density distribution in the reference file

should be that that would be measured normal to the beam. The cosine effect that is due to the specular nature of the coating will be automatically included in the calculation.

Scattering and Surface Roughness

Incoherent scattering is a phenomenon where light is lost to the system in non-specular directions. The major culprit in optical coatings is surface roughness and there are some tools that help in calculating the magnitude of the effect. Because roughness is random and fractal it is impossible to specify it precisely, and statistical measures are used. A common one is the root mean square deviation from a perfect surface, denoted by σ. To improve the characterization of the surface we can add an idea of the correlation length of the roughness.

There are two tools that yield some idea of the effect of roughness. The simplest assumes that the roughness is extremely small and either very short range with a correlation length much less than a wavelength, or rather longer range, with correlation length rather greater than a wavelength. Both are handled by introducing a transition layer at the rough surface that is 2σ in thickness. The layer is given the Medium attribute and is entered as Scatter(s) for the short range condition or Scatter(l) for the long range. Scatter(s) represents the condition simply as a graded layer with no incoherent loss, but Scatter(l) includes loss to represent what is lost to the system through the scattering. Note that the model is very approximate and may be still less reliable at oblique incidence.

The second tool is available in the Analysis collection and performs some limited calculations of the angular distribution of scattered light following the model of J. Merle Elson. More details are given in the Analysis and Design Tools chapter.

We emphasize again that calculations involving surface statistical parameters are necessarily very approximate and can never present an accuracy similar to that for specular interference effects. The results should be treated as no more than a very rough indication.

Polarization Maintenance

In some applications it is important that an optical coating will not perturb the polarization of an incident beam in either reflection or transmission. At normal incidence, a thin-film coating on a surface, where all materials are isotropic, will not perturb the incident polarization beyond changing its handedness in reflection. This is no longer generally true at oblique incidence. If there is any difference between the p and s-performance then the polarization state of the incident light will be perturbed in both reflection and transmission unless it is linearly polarized parallel to either the p or s-direction. This perturbation implies that a fraction of linearly polarized incident light will appear in an orthogonal mode. This phenomenon is sometimes called polarization leakage but this is a term that is already used in the Essential Macleod in respect of a ray out of the principal plane of incidence and calculated in vStack. We therefore term this effect polarization coupling. A complementary term that is a measure of the extent to which the polarization of the incident beam is preserved, is polarization maintenance.

These parameters are typically measured by placing a polarizer in the incident beam aligned at 45° to the p and s-directions, and an analyzer in the emergent beam. The analyzer is first aligned parallel to the input polarization to give the signal level and then

orthogonal to it to give the leakage. The leakage irradiance, in the second orientation, divided by the sum of the leakage and the signal in the first, expressed as a percentage, is then the measure of polarization coupling. The irradiance in the signal orientation divided by the sum of the irradiances, again expressed as a percentage, is then the measure of polarization maintenance.

The polarization maintenance parameter can be calculated for Designs (without thick layers) and for vStacks by selecting Transmittance PM or Reflectance PM in the parameter dialogs. It can also be used as a target for refinement.

Coating design derivation

There are two principal reasons for the derivation of a design to be required. The first is the straightforward need for a coating that must perform a given task. The second is sometimes called reverse engineering. An actual coating performance has been measured and the structure of the coating must be determined. Frequently this is associated with difficulties that have occurred in the attempted production of a known coating design. Both of these are quite similar operations.

Calculation of the properties of a given design is straightforward because performance is a single-valued calculable function of the parameters. Derivation of a design, however, is much more difficult because there is no direct path back from performance to design parameters and no single-valued result. How then can we proceed?

We recognize that knowledge, skill, judgment, experience, instinct and luck are all attributes of the successful designer. Most of these are subjective and therefore difficult to replace by a computer no matter how efficient and powerful. However the computer can help to remove those parts of the task that do involve intensive or tedious calculation and the speed at which evaluations can be performed make automatic design feasible in many cases.

The computer can carry out performance evaluations very quickly. Imagine that the computer makes changes in the layers of a design and each time a change is made the performance is evaluated. A change that results in improved performance can be retained while a poorer one is discarded. In this way a given design may be gradually improved. From the pattern of results it may be possible to increase the rate of improvement. This is the technique of refinement where a starting design that is short in performance can be improved to meet a requirement. Now imagine that we have a design that is much more remote from an acceptable result but we have, however, a method of increasing the complexity of the design by adding layers in such a way that the successively refined performance continually improves. Eventually we build a design that is much more involved than the starting design but that meets the requirements. This is the process of synthesis. Refinement and synthesis have great similarities. Refinement can usually be relied on to achieve its potential, while synthesis rather less certain but can, on occasions, achieve an astonishing degree of success. Processes classified as refinement would be ones that we would use routinely, while synthesis would be for times when we are hard pressed and without much inspiration. Reverse engineering will make much use of refinement and rather less of synthesis.

The Essential Macleod is well supplied with synthesis and refinement techniques. Two synthesis methods are supplied. The first is based on a method we call Optimac that

incorporates many different procedures for increasing design complexity. The program constantly evaluates itself and quite ruthlessly discards procedures that are proving ineffective as the synthesis proceeds but encourages those that are working well. Clearly the volume of calculation in a synthesis procedure is greater than that required in refinement, and so the time involved in the achieving of a design must be rather longer. For routine work therefore, refinement based on the nonlinear simplex technique is recommended. For rather less easy refinement problems where time is not so pressing there is simulated annealing. Then there are two techniques that include guidance from derivatives. Conjugate Gradient and Quasi-Newton can often present surprisingly fast convergence on an optimum design. Optimac itself can also be used for refinement and it is very efficient in that role.

The second synthesis method is Needle synthesis. This method looks for a place to insert a new layer by calculating the derivative of the merit figure with respect to layer thickness for a zero thickness layer. The zero thickness layer is moved throughout the existing layers. The point at which the merit figure derivative reaches its largest negative value is the insertion point of the new layer. After all the new layers have been inserted (the needle method may insert more than one layer), Conjugate Gradient refinement is performed. This increases the thicknesses of the new layers to non-zero values. Also, the other layers will have their thicknesses adjusted by the refinement as would happen if a design was being refined.

None of these methods removes the need for skill, and it is easy to show that there is no procedure that can do that at the present stage of development of computers. Nevertheless the techniques supplied here are powerful tools and they help enormously. It is clear, though, that we are a very long way from the day when ability, interest and application will become irrelevant.

Work Data Management

In normal use of the Essential Macleod, you typically work with a single materials database, and a single set of reference data (including scripts if the Function option is installed). For various reasons, you may want to separate your data into different regions. This may be, for example, because you are a consultant and need to keep all data for one client completely separate from data for another client. The Jobs facility provides this capability. A Job is represented by a folder name and contains a Materials folder, a References folder (including scripts) and a Designs folder. A Job can be created, opened and closed. When a Job is created, you enter a folder name – this is the name of the Job. Typically this folder will be stored in the My Documents\Thin Film Center\Jobs folder, but you can locate it anywhere on the computer including a removable drive. A new empty materials folder is created. A new references folder is created and all reference data and scripts are copied from the main references folder to the new folder. A new designs folder is also created. The Essential Macleod's parameters are set so that these new folders are the default folders for loading and saving information. To show that a Job is open, the title bar of the Essential Macleod shows the name of the open Job.

A Job can also be closed. This means that the Essential Macleod will be reset so that it uses the normal materials folder and the normal references folder. The default location for designs etc. will be changed back to what was last used when no Job was open. The

Essential Macleod title bar will just show “Essential Macleod” to show that no Job is open.

Maintenance of Materials Data

The thin films that make up the coating and the incident and emergent media are all characterized by a refractive index, *n*, and an extinction coefficient, *k*. These are discussed in greater detail under Conventions above.

Real materials, with the exception of free space, suffer from dispersion that is a variation of *n* and *k* with wavelength. This variation must be taken into account whenever the wavelength is changed during a calculation. Ideal dielectric materials in their transmittance region exhibit what is known as normal dispersion. Normal dispersion is predictable from straightforward harmonic oscillator theory and there are several expressions that can be used to fit the behavior. Ideal metals have quite different behavior that depends largely on free rather than bound electrons although again there are ideal expressions that exhibit ideal metallic behavior. Real materials, and especially thin film materials, are somewhat more complicated than these ideals and the validity of the various formulae that exist is limited.

Refractive index data may be stored in several different ways: as Sellmeier coefficients, as Cauchy coefficients, as Drude coefficients, as Lorentz coefficients, as Drude-Lorentz coefficients, or a table of data. The extinction coefficient part may be stored as a table, a set of Cauchy coefficients, a pair of exponential coefficients or may be declared as always zero. For Drude, Lorentz, Drude-Lorentz, the extinction coefficient information in an integral part of the coefficient set, so there is no separate extinction coefficient definition. When tabular data are used, values needed during calculations are derived by linear interpolation. The data can be given at any series of wavelengths which do not need to be equally spaced. Where the values are changing rapidly, for example, the density of data can be greater.

Maintenance of the material optical constant data is therefore an important task that is the function of a major division of the package. Data may be examined and displayed. It may be edited, added to or deleted. Fresh materials may be introduced. The optical constants may be automatically derived from spectrometric measurements. Many different independent databases of materials may be maintained, even with different systems of units, and with easy transfer of data from one to the other.

Analysis and understanding

Often the sequence of layers that make up a design is not enough. We need also to understand how the design works and where the critical regions lie where particular attention to detail like roughness or contamination is required. This is the purpose of the group of tools known as Analysis. Admittance loci, electric field plots, potential transmittance, symmetrical periods, and the like are included.

Combinations of coatings

Frequently the final product will not be one single coated surface but a combination of surfaces, some coated, some uncoated. For example a filter with a cemented cover over it

will consist of four surfaces separated by optical material, only one of which is coated. Or perhaps there will be antireflection coatings on the outer surfaces. There may be as many as forty surfaces in a compound lens consisting of elements of different optical constants, all with antireflection coatings. Both the Stack editor and Design editor deal with this situation. A virtually limitless, within the capacity of the computer of course, number of different media, each bounded by two surfaces, either parallel or wedged, can be accommodated.

Packing Density

Materials in thin film form rarely have bulk properties. The primary reason for this is their microstructure that is seldom bulk-like but usually exhibits a pronounced columnar morphology. The most unfortunate features of the columnar microstructure are the pore-shaped voids between the columns and they are the main culprits in reducing film packing density, which in turn affects the optical, and other, properties. The Essential Macleod uses packing density as a vehicle both for simulating the effects of a change in packing density, in practice this could be due to a change in deposition conditions, but also as a convenient way of introducing variable refractive index.

The model that is used for the variation of optical constants as a function of packing density is a very simple empirical relationship first proposed by K Kinosita and M Nishibori. (*Porosity of MgF2 films - evaluation based on changes in refractive index due to adsorption of vapors. J. Vac. Sci. Technol., Vol 6, pp 730-733, 1969*) that has since been shown to represent very well the behavior of many dielectric films. (Since the relationship is single-valued and continuous it would be straightforward to calibrate the packing density so that it represented a more involved relationship.)

$$p = \frac{Volume\ of\ solid\ part\ of\ film}{Total\ volume\ of\ film}$$

and the refractive index of the film is given by

$$n = (1 - p)n_v + pn_s$$

where n is the composite index, n_v is the index of the material filling the voids and n_s is the index of the solid part of the films, the columns.

In the Essential Macleod n_v is given by a void material and a void density. That is, the void material can be specified, and it can be defined to occupy a certain proportion of the void space (the remainder of the void space is occupied by air, n = 1.0). This allows effects such as partial saturation with water to be modeled. The refractive index of the complete void is given by $n = (1 - p)n_v + pn_s$, where n_v is the refractive index of the unoccupied void (1.0), n_s is the refractive index of the void material and p specifies the amount of void space occupied by the void material. When p = 1, the whole void space is occupied by the material. When p = 0, there is no void material in the void space. The refractive index of the layer is therefore given by

$$n = (1 - p)[(1 - f) + f n_v] + p n_s$$

where n is the composite index, p is the packing density of the layer material, f is the packing density of the void material, n_v is the refractive index of the void material and n_s is the refractive index of the layer material.

As well as permitting refinement in terms of refractive index, packing density is particularly useful in reverse engineering and in simulating inhomogeneous layers.

The packing density can be applied to both the real and imaginary parts of the complex refractive index (refractive index and extinction coefficient), or to just the refractive index leaving the extinction coefficient unchanged. This is controlled by selecting General from the Options menu. Next, click on the Designs tab. To have packing density control the extinction coefficient as well as the refractive index, check "Use Packing Density to adjust Extinction Coefficient". By default, extinction coefficient is not adjusted by the packing density.

Units in the Essential Macleod

Most of the variables in the Essential Macleod, wavelength, frequency, magnitude etc., have units. These units can be chosen virtually at will.

Since the same user may sometimes want to work in terms of wavelengths in microns and sometimes in terms of nanometres and so on, the units are tied to the materials database. Each different database may have completely different units. Since materials data are actually held in generic units (although the user need not know this - more about it later in this section) there is no need to convert the materials data when modifying the working units.

The package can be thought of as calculating in terms of the fundamental set of SI units. Wavelength is a unit of length therefore it is in metres. Frequency is in hertz. Time is in seconds. Physical thickness is in metres. Using appropriate factors, these fundamental units may then be converted into a set of display units. The convention for the factors is that they should be expressed as *the ratio of the desired unit to the fundamental unit*., and they are therefore known as scale factors.

A list of scale factors for most of the possibilities is given in a following table but it may also be helpful to work through several of them to illustrate how they may be derived.

Useful constants and prefixes	
Velocity of light	2.99792458×10^{8} metre per second
Planck's constant	$6.626070040\times10^{-34}$ joule second
Electron volt energy	$1.6021766208\times10^{-19}$ joule
Some prefixes	Factor of 10^{-18} : atto with symbol a Factor of 10^{-15} : femto with symbol f Factor of 10^{+12} : tera with symbol T Factor of 10^{+15} : peta with symbol P Factor of 10^{+18} : exa with symbol E

The first and most important rule is that the conversion must be through a linearly proportional relationship. Thus wavelength may be converted only into those quantities that are linearly proportional to wavelength and so on.

Wavelength units are very straightforward. For example, 1nm is 10^{-9} metre and so the scale factor for nm is 10^{-9}m divided by 1m, that is 10^{-9}.

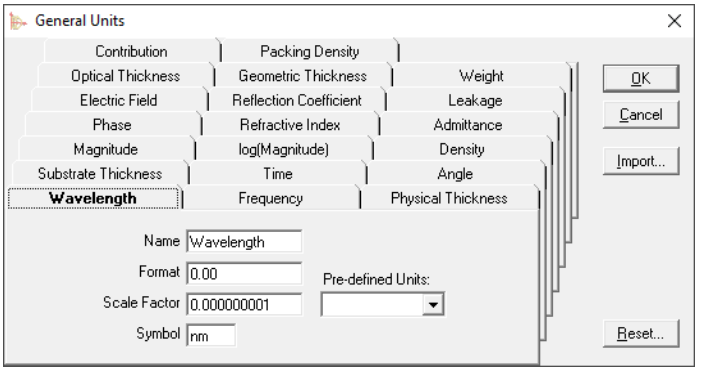
Next we consider conversion from frequency in Hz to wavenumber in cm^{-1}. This is a little more involved. Wavenumber is short for the number of waves per unit of length. This is linearly proportional to frequency so that the conversion is possible. Light travels a distance equal to its velocity in unit time and the number of waves in this distance is given by the frequency. Light with one wave per centimetre, therefore, has 100 waves in one metre and $100\times2.99792458\times10^{8} = 2.99792458\times10^{10}$ in 2.99792458×10^{8} metres. That is its frequency must be 2.99792458×10^{10} Hz. The scale factor is therefore this quantity divided by 1Hz, i.e. 2.99792458×10^{10}.

Now we look at conversion from frequency in hertz to photon energy in electron volts. One electron volt has an energy of $1.6021766208\times10^{-19}$ joule. We divide this by Planck's constant to find the frequency in hertz, that is $2.4179892623\times10^{14}$ Hz. The scale factor for Hz to eV is therefore $2.4179892623\times10^{14}$.

Category	Name	Scale Factor	Symbol
Wavelength	Wavelength	1E-09	Nm
Wavelength	Wavelength	1E-10	Å
Wavelength	Wavelength	1E-06	µm
Frequency	Wavenumber	2.99792458E+10	cm-1
Frequency	Energy	2.4179892623E+14	eV
Frequency	Frequency	1E+15	PHz
Frequency	Frequency	1E+12	THz
Frequency	Frequency	1E+09	GHz
Frequency	Angular Frequency	1.59154943092E+14	rfs-1
Time	Time	1E-15	Fs
Physical Thickness	Thickness	1E-10	Å
Physical Thickness	Thickness	1E-09	Nm
Physical Thickness	Thickness	1E-06	µm
Physical Thickness	Thickness	1E-03	Mm
Note:	key codes for the symbol µ		Alt+0181
	key codes for the symbol Å		Alt+0197

Angular frequency may also be useful at times, particularly when dealing with short pulses. We can use units of radians per femtosecond, rfs-1, for example. In hertz this is $(1/2\pi)\times10^{15}$Hz.

Access to the definitions of the general units is available only when no files are open. The **Options** menu for the Application window has an item **General Units...**. General units are those that are used in the performance calculations.



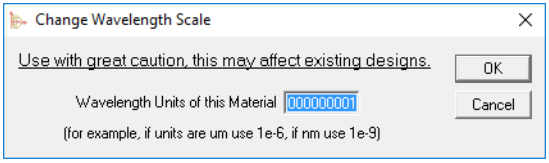
Once the units have been defined for a particular database they will remain as defined until intentionally changed. Materials data are stored in terms of generic wavelength units.

Several units have a selection of pre-defined units available. Click the dropdown arrow of the **Pre-defined Units** list to see the options available for the particular unit.

You can copy the unit definitions from a materials database into the current materials database by clicking the **Import…** button. A folder chooser will be displayed. Select the folder containing the desired units, and click OK. The units in the selected database will be copied into the form. You will not be able to select OK in the folder chooser if the selected folder does not contain units definitions.

The materials database holds the optical constants of materials in terms of wavelength (but can display the data in terms of frequency). As the wavelength or frequency units are changed from one type to another the display of optical constants and the calculations all follow. No changes need be made to the materials database. Similarly when one material is imported into another database, any necessary unit conversion is completely automatic. The data is actually stored in generic units and the program converts backwards and forwards between these generic units and the current display ones. Any new material that is entered should have data given in terms of the current wavelength units, whatever they are, and then the conversion to the generic units of the database will be completely automatic. It may be, however, that data to be imported is given in some alternative units.

The current ones might be microns and the data might be in terms of nanometres for example. Conversion before entry is tedious and therefore it is possible to enter data in any wavelength units. If the units are not the current ones then a scale factor must be given. Use the **Wavelength Scale...** command in the **Edit** menu for an individual material. The scale factor should be exactly that that would be entered in the **General Units** dialog. It is one unit of wavelength expressed in metres.



Line styles in the Essential Macleod

The default appearance of all plotted lines is consistent throughout the package. As drawn, all lines are full lines. They are color coded as black for normal incidence, blue for s-polarization at oblique incidence, red for p-polarization at oblique incidence and green for mean polarization at oblique incidence. The style and color can be changed in the normal way and broken lines are included in the available choices.

Color

The color of any object is a subjective response that varies from one individual to another. In order to permit unambiguous quantitative determination of color, standard observers have been defined. Color measurements and comparisons are therefore normally made with respect to the standard observers, that in turn have been created after many different measurements on many real observers. The two most common observers have been defined by international agreement and consist of three color matching functions that are measures of the amount of three defined primary colors that are necessary exactly to match pure spectral colors, each of 1W radiant power, across the

visible region. These functions are known as $\bar{x}$, $\bar{y}$ and $\bar{z}$ and they correspond to color matching using the red, green and blue primaries respectively. There are two internationally agreed sets of standard observer color matching functions, the CIE 1931 set and the CIE 1964 set. These sets are quite similar but the 1964 set is intended better to represent fields subtending angles of 10° while the CIE 1931 set corresponds to 2°.

Given the color matching functions for spectral lines, the amounts of the three primary colors required to match any light source can be calculated simply by decomposing it into its spectral distribution, multiplying by the appropriate tristimulus values and integrating. These amounts of primary colors are known as the tristimulus values. Since thin film coatings are not self-luminous they must first be illuminated by a light source and then the tristimulus values of either the light reflected by the coating or that transmitted, can be calculated. Coating color calculations therefore begin by finding the tristimulus values, *X*, *Y*, and *Z*, for the coating and the light source. Then the raw tristimulus values may be manipulated into sets of three coordinates in various defined versions of color space. Simple normalization to give a sum of unity yields the Chromaticity Coordinates, for example.

The different coordinate systems presently available for calculation by the Essential Macleod are Tristimulus, Chromaticity, CIE L*a*b*, CIE L*u*v*, CIE L*u'v', Hunter Lab, CIE1960 uv, Correlated Color Temperature and Dominant Wavelength. These coordinate systems are hard coded in the program and can not be changed by the user. Color Rendering Index is also calculated. Color difference in the CIE L*a*b* coordinate system can also be calculated using either the CIE76 method or the CIEDE2000 method.

Standard light sources that are supplied with the program are CIE defined and consist of illuminants A, B, C, D55, D65, D75 and equal energy. Standard observer color matching functions supplied are the CIE 1931 observer and the CIE 1964 observer.

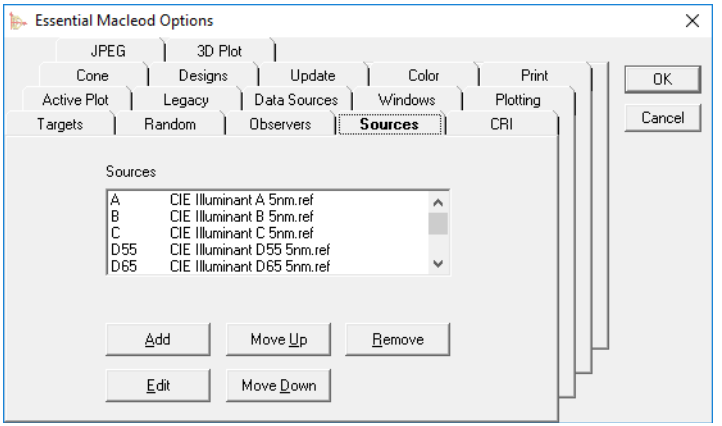
The light sources and the standard observers are not hard coded and can be supplemented or changed by the user. They consist of a series of reference files in the reference folder (defined in the General Options dialog box). The light sources are defined by the file sources.src in the reference folder and the observers are defined by the file observers.obs also in the reference folder. These files are maintained using the General command in the Options menu. The sources are maintained on the Sources tab and the Observers are maintained on the Observers tab. You can add, delete, edit and change the order of appearance of sources and observers.

To add a source, place the spectral response in a reference file in the reference folder. The format consists of a header

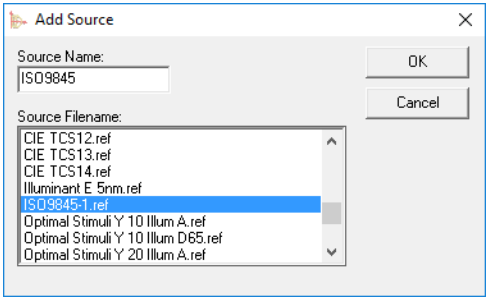
WAVELENGTH<Tab>REL OUTPUT

followed by records each consisting of a wavelength in nm and relative output separated by a tab character. *Note that the wavelength should always be in nm even if the general units being used are different.* An easy way of entering the information is by setting it up first as a table and then creating a reference file from it using the **Create Reference...** command in the **File** menu.

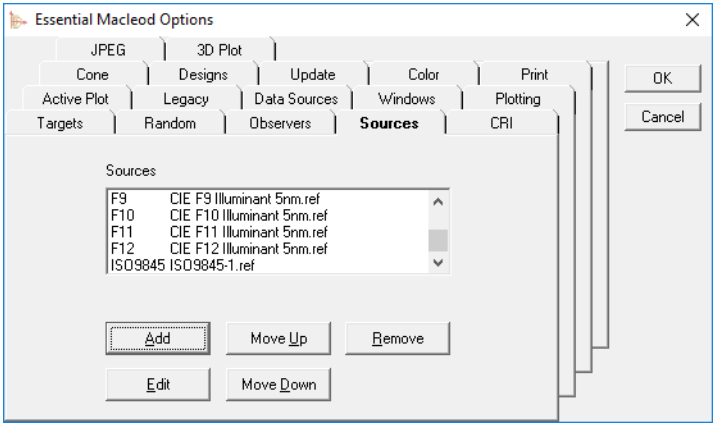
Once the reference file has been created, select General from the Options menu and click on the Sources tab:



Click the Add button.

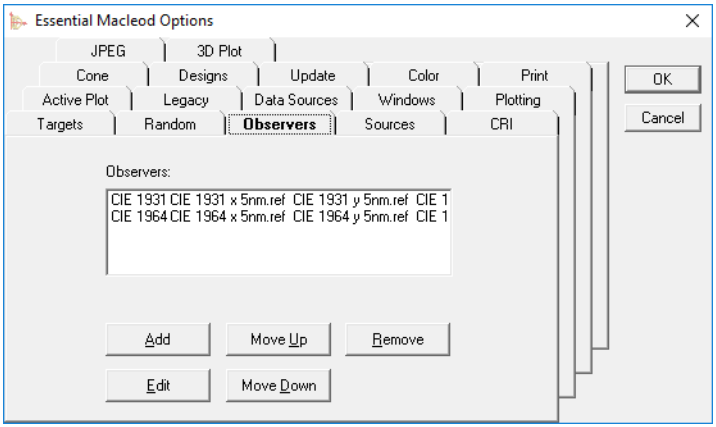


In the Source Name field enter the name of the source as you would like to see it displayed. In the Source Filename field, select the reference file that contains the new source data, and then click OK.

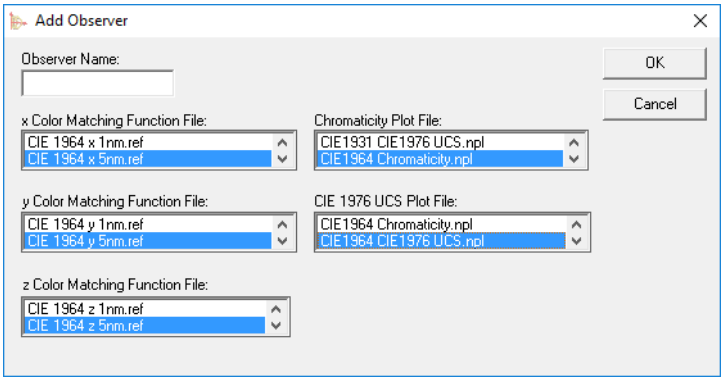


The Add Source dialog will now close and the Source list will be updated with the new source. Click OK to save the new source information and close the General Options dialog.

More information is required for Observers. Three files must be defined which give the x, y and z color matching functions. Optionally a plot file showing the boundary of chromaticity space can be defined for the observer and also a plot file showing the boundary of CIE 1976 UCS space can also be defined. W*avelengths for the x, y and z color matching functions must be in nm.* Select General from the Options menu and then click on Observers.

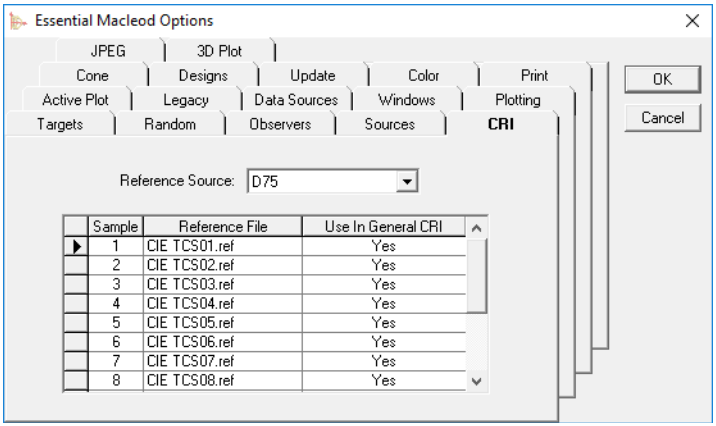


Select the CIE 1964 observer and click Edit.



The Edit Observer form allows you to specify the files needed to define an Observer.

For Color Rendering Index, the test color sample files are held in the References folder. The standard files supplied with the software are named CIE TCS01.ref to CIE TCS14.ref. The calculation uses up to 14 test color samples when calculating Color Rendering Index. The samples used for determining the general Color Rendering Index may be specified by the user, and are normally the first eight test color samples.



Use the **Browse** button to select the reference file that defines the reference source spectrum for the color rendering index calculation. To change the file used for a test color sample, double-click in the **Reference File** cell and select the file in the file chooser that appears. To include or exclude a sample from the general coloring rendering index calculation, click on the cell in the **Use In General CRI** column.

Derivatives in the Essential Macleod

Derivatives up to the third order of most performance parameters can be calculated in the Essential Macleod simply by entering the appropriate order number against derivative in the Vertical Axis section of the Performance Parameters dialog box (described later). *These derivatives are with respect to wavelength.*

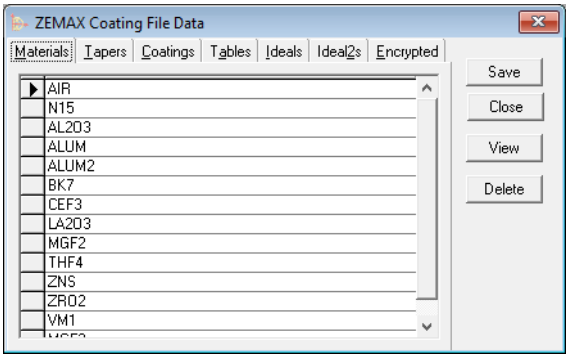
The derivatives are calculated from analytic expressions for each of the performance parameters. The derivatives of the optical constants defined by tables are determined numerically. The optical constants in the package are linearly interpolated from tables and so there can be sudden changes in slope that would show up clearly in the derivatives of performance. Therefore the slope of the optical constants is smoothed around the corners to avoid any sudden change within the calculation range. The region over which this smoothing takes place is defined by the Wavelength Delta Factor. The first derivative of the optical constants is given by the difference between the optical constant at (1 + WavelengthDeltaFactor) * Wavelength and the optical constant at (1 – WavelengthDeltaFactor) * Wavelength divided by WavelengthDeltaFactor * Wavelength.

To modify the definition, select **General** from the **Options** menu and then select the **Designs** tab. **Wavelength Delta Factor** gives the interval used for determining the first derivative of the optical constants. It is difficult to determine reliable values for the second and third derivatives and so these values are set to zero. Generally, the optical constant derivatives have negligible effect on the derivatives of the performance parameters

Exporting coating designs to Zemax

Coatings are important features of optical components and systems and the Zemax series of lens design packages includes coatings in its performance assessments. Zemax does not have any facilities for generating or editing designs. It stores and reads the designs together with data on materials from a special coating file that has a prescribed format. In particular, the layers in the designs must be specified in terms of optical thicknesses at a given reference wavelength, or in terms of physical thicknesses. Zemax also provides the ability to use the performance of a coating rather than the definition of a coating. The Essential Macleod includes an editor for the Zemax file that makes the transfer of coating designs or their performance to Zemax extremely simple and straightforward, and, more important, reliable. The user need not be concerned about the special formats that are required nor about the constraints on total numbers of layers or material information. All of this is checked automatically.

To activate the Zemax coating file editor the current file must be opened. The command for this is **Load Zemax Coating File...** in the **Tools** menu for most documents. A new Zemax coating file can be created by selecting **New Zemax Coating File** in the **Tools** menu. The appearance of the main window of the Zemax editor is shown below.



The window has seven tabs, materials, tapers, coatings, tables, ideals, ideal2s and encrypted. The coatings are defined by the name of the design file from which they were exported. The materials are defined by the names that they had in the materials database from which they were originally extracted. Tapers, ideals and encrypted files are defined by editing the file directly. Design, material and table names are converted to upper case before the data are written to the Zemax file. Once they have been written, these names may not be edited. The editing operations are limited to deletion or addition. This is intentional. The data are intended for use in another application and have been exported. Editing existing data may invalidate already performed calculations so editing should be carried out only under special circumstances with an understanding of the extent of the consequences.

To examine, but not edit, the data stored for any of the materials, tapers, designs, tables or ideals either double-click on the appropriate name or select the item and click **View**. A table will appear listing the stored information.

To add a new design, first make the design window active. Then select **Add to Zemax File** in the **Export** submenu of the **File** menu.

There are five options in the submenu, **Relative Thicknesses Without Substrate**, **Relative Thicknesses With Substrate**, **Absolute Thicknesses Without Substrate**, **Absolute Thicknesses With Substrate**, and **As Performance Table….**

Choosing one of the **Relative Thicknesses** options will export the design with thicknesses defined as optical thicknesses. The actual design will be given by the combination of the layer thicknesses and the reference wavelength defined in Zemax. Designs can only be exported this way if they are defined in terms of optical thicknesses in the Essential Macleod. Choosing one of the **Absolute Thicknesses** options will export the design with thicknesses defined as physical thicknesses. The coating will have the same performance regardless of the reference wavelength defined in Zemax. Choosing the **As Performance Table** option will export the reflectance and transmittance magnitude and phase data for s and p polarization for a user-defined range of incident angles and wavelengths.

Opaque layers and substrates can be included in the Zemax coating designs but in a way that is a little different from the Essential Macleod and needs some explanation.

The normal Zemax coating design is a series of thin and reasonably transparent films only. These structures are essentially transmitting assemblies and the substrate is automatically designated in the Zemax system design so it is not required as part of the coating. However, if the coating contains an opaque metallic film such as a thick layer of aluminum then it will have zero transmittance and its function will be that of a reflector. Such thick opaque films require special treatment. In the Essential Macleod special algorithms are activated automatically when necessary without the user even being aware of them. In the Zemax calculations, such opaque layers are treated as a massive opaque substrate, *but the opaque substrate must be included as a final dummy layer in the design*.

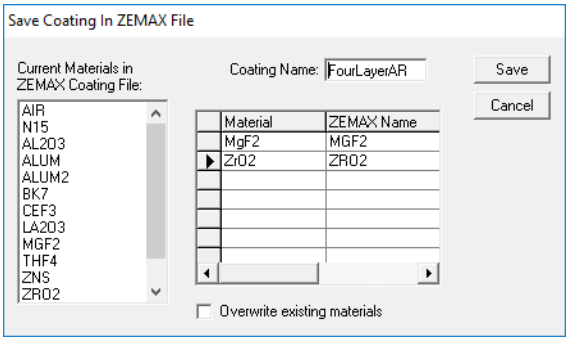
In the Essential Macleod the design of a front surface mirror based on, for example, aluminum, may be specified in two different ways. Either the aluminum may be defined as the substrate or the final layer of the design may be a thick aluminum layer. In Zemax this design will be handled in the former way but the design will be specified in the latter way.

When passing designs of reflectors to Zemax, then, if the films include the opaque layer as the final layer, then the submenu choice should be **Without Substrate.** If the layers are essentially transparent and the substrate is opaque then the submenu choice should be **With Substrate**.

Since it may not always be obvious whether or not the substrate should be included it is arranged that an included substrate has zero thickness so that if passed incorrectly as a film to Zemax rather than a substrate, it will have no influence on the performance of the design.

Once the command is activated, several things happen. First, the materials list in the design is checked against the materials already in the Zemax coating file. The list together with the name of the coating is presented in a dialog box that appears. The coating name can be edited at this stage. The edited name will be used in the Zemax file but this will not change the existing design name. Clicking the Save button saves the coating together with any materials that are not already in the Zemax file. Should,

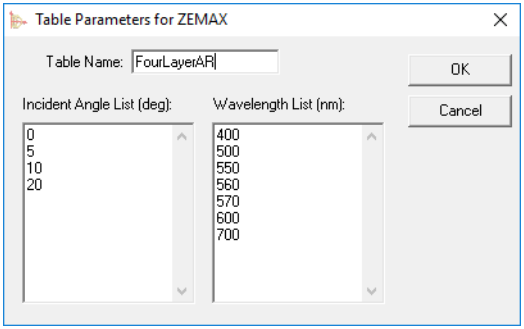
however, the name of the design correspond to one already in the Zemax file then a warning message will appear and the design will not be written until the name is edited to something unique. Materials, too, that already exist in the Zemax file are checked more thoroughly at this stage. If their data does not correspond to that in the current material file then, again, the file will not be written. There are now two choices. The Zemax name may be altered - type in the new name in the list over the old - and this altered name will appear in the Zemax file. Alternatively, the existing material may be overwritten.



Zemax coating designs are limited to a maximum of 400 layers and coating materials to a maximum of 120 points. These limits are also checked at this stage and appropriate warnings generated if necessary.

It is a good plan to maintain a special materials database for Zemax alone. Quite a few of the materials in the regular Macleod databases have more than 120 wavelength points and must be edited down to this number before they can be passed to Zemax. This is best done in a dedicated database.

When a design is exported **As Performance Table**, you will be asked to enter the set of incident angles and wavelengths for calculating performance in the following form:

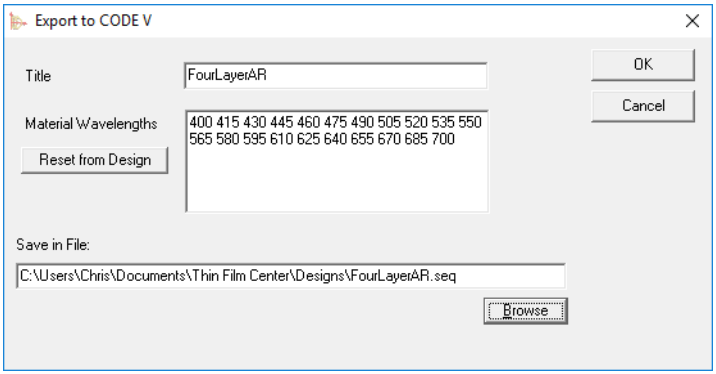


Incident angles and wavelengths do not have to be equally spaced. Once you have entered the information, click OK. This will cause the performance data to be calculated and added to the Zemax coating file.

Exporting data for CODE V

CODE V is a lens design package produced by Optical Research Associates. A CODE V model can include coatings. The Essential Macleod generates sequence files that contain definitions of coatings. These sequence files can be read by CODE V and cause the coating definition to be loaded into CODE V. For information on using sequence files, please consult the CODE V user's manual.

To export a design for use in CODE V, select CODE V Sequence File from the Export menu in the File menu of a design. A form will appear as shown below.



There are three parameters for the Export: The title to be used for the coating, the list of wavelengths for which n and k data are to be provided and the filename for the sequence file. CODE V permits definition of up to 100 wavelengths for refractive index dispersion data. Since the Essential Macleod is unlimited in the number of data points for refractive index data, you are required to specify the individual wavelengths for which refractive index is to be generated. **Reset from Design** will create a list of 100 equally spaced wavelengths from the max and min values of the wavelength axis used for performance calculations. This list can then be edited to produce the required wavelengths if necessary. Once the parameters have been completed, click **OK** to export the data.

Exporting data for FRED

FRED is an optical system modeling package that can include the effects of coatings. To export a coating design to FRED, select FRED from the Export sub-menu of the File menu of the Design window. You will be asked to provide a filename for the file that will contain the coating data. Material data is automatically included in the file. Please see the FRED user manual for information on loading the coating data into FRED.

Exporting coating designs to VirtualLab

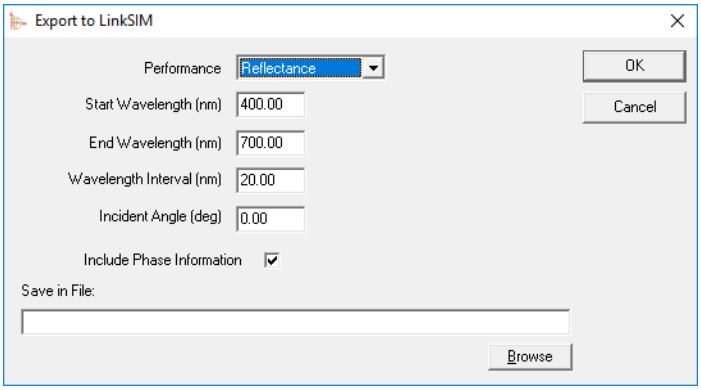
The VirtualLab package integrates several toolboxes allowing the analysis of systems, design of diffractive optical elements, design of beam shapers, analysis of gratings, analysis of laser resonators as well as the shaping and homogenization of LED light. To

export a design to VirtualLab, make sure the design is active and then select Export in the File menu. This will export a VirtualLab Coating Data File (*.vlct) containing layer parameters and materials data. Importing the design into VirtualLab uses the Import Macleod Coating Data item in the VirtualLab Tools menu of the Coating Catalog.

Exporting data for LinkSIM

LinkSIM is an optical communication system simulation package which includes an object-oriented topology layout facility, a waveform simulation engine, and display and analysis tools. It is used to design optical communication links and simulate them to determine their performance given various component parameters. The Export feature permits the performance of a coating design or stack to be included in the simulation.

To export the data, click LinkSIM Filter File in the Export sub-menu of the File menu. This will display the dialog shown below:



The data file can contain the reflectance or transmittance data. The wavelength range for the data are specified by Start Wavelength, End Wavelength and Wavelength Interval. The data will be generated for the specified Incident Angle. For Designs, you can choose to include phase information as well. Click Browse to use a file chooser for selecting the destination file. For data at oblique incidence, the export will generate two files, one will have "_p" added to the filename and the file will contain p-polarization data. The other will have "_s"added to the filename and the file will contain s-polarization data.

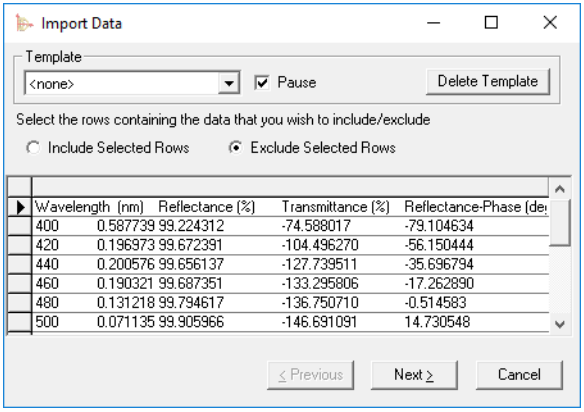
When data is being exported from a Stack, the calculations will include any bandwidth and cone settings as specified for the Vertical Axis parameters.

Please see the LinkSIM documentation for instructions on how to use the file data in a LinkSIM simulation. LinkSIM has now been incorporated into the OptSIM software package

Importing Data

When data are imported from external text sources, a data import tool is used. This tool allows you to specify the structure of the data, exclude unwanted from the import and specify the meaning of the data to be imported. The settings used in the import data

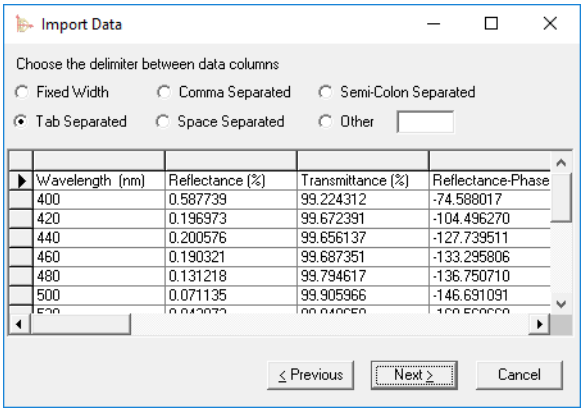
window can be saved as a template for future use. This makes repeated data import from the same data source much quicker. Multiple templates can be saved so that layout of different data sources can be retained in the Essential Macleod. The data import tool is triggered in many ways including opening a file with an extension that is not of the Essential Macleod set of file extensions and pasting textual data into an Essential Macleod window. The figure below shows the first screen shown when opening a text file containing tab-separated data. The import data window can be resized to show more data if desired.



On this screen, you can exclude unwanted data from the import. Typically, this will be unwanted headers. In this case, we are going to keep the headers for use later. You can either select the rows that are to be included or select the rows that are to be excluded. Inclusion/Exclusion is controlled by selecting the appropriate option above the table.

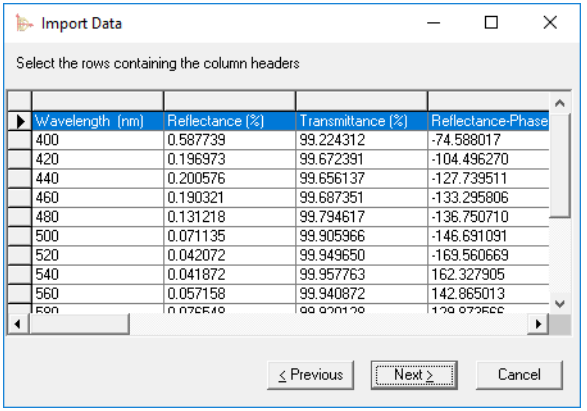
At the top of the screen, a previously saved template can be selected, or, if a template was previously saved with the default option checked (see later) it will automatically be selected. When a template is selected is can be deleted used the **Delete Template** button. Otherwise, the template can be used by clicking the **Next >** / **Finish** button. If the **Pause** option is checked, the button will be labeled **Next >** and the import will pause at the final screen. If the **Pause** option is unchecked, the button will be labeled **Finish** and the import will complete without further interaction.

When no template is selected, click **Next** to move to the next screen.

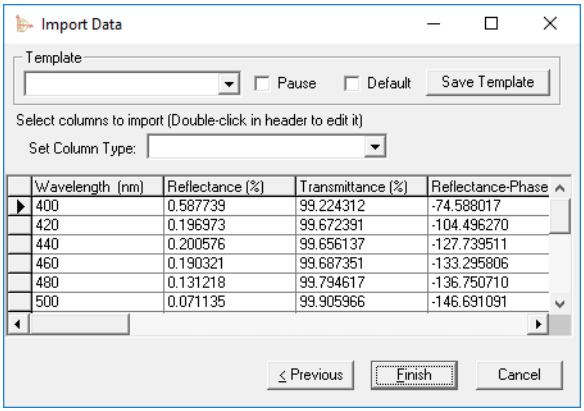


This screen is used to specify the separators between the columns of data. If the data is fixed width, you can specify where the data is to be separated by clicking at the appropriate location on any of the data rows. Once you have clicked, the data will be reformatted with one extra column. If a column is incorrect, double-clicking in the header of a column will merge it with the column to the right.

Once the columns are correctly separated, click **Next** to move to the next screen. The next screen depends upon the import being performed. In this example, a data file is being opened and the next screen allows you to specify that one or more rows in the file contain header information.

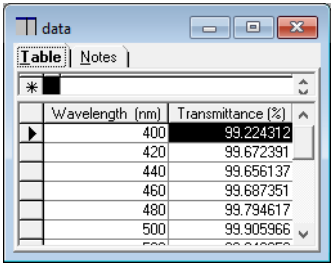


The headers are specified by selecting the rows containing the header information. Click **Next** to continue.

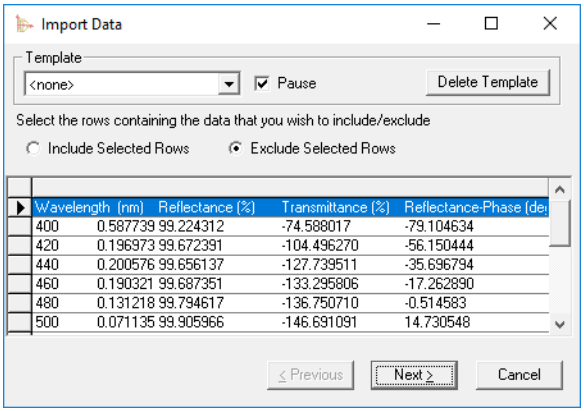


The next screen allows you control which columns are imported. For each column, select the column by clicking in the column header. In **Set Column Type**, choose **Import** or **Ignore**. If you choose **Ignore**, the column header will be set to Ignore. You can also edit the column headers by double-clicking on the column header. This will display an edit box where you can change the header text. Click **Finish** to complete the import. The figure below shows the completed import after the blank columns were ignored.

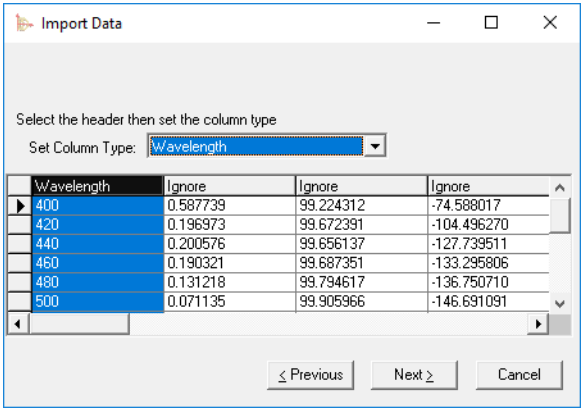
The Template section allows the previously defined formatting of the import data to be saved for later use. You can either type in a name for the template or overwrite an existing template. Checking the **Pause** option will cause Pause to be automatically selected when the template is selected on the first screen. Checking the **Default** option will cause the template to be automatically selected when the import editor is started.



For data that are to be pasted into editors where the columns have specific meanings, the import process is slightly different. Here we show the import of the same data into the Design Targets editor. The data have been placed on the clipboard and **Paste All Targets** has been selected from the **Edit** menu of the Target editor.

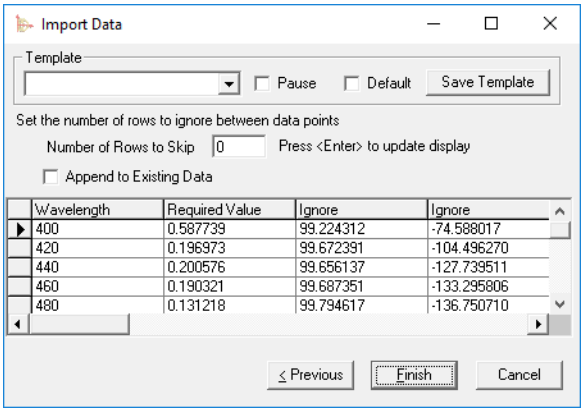


In this case we do not want the headers from the file, so the header line has been selected so that it will be excluded from the import. After clicking **Next** to set the column separators and then clicking **Next** again, the type of the data in each column is specified.



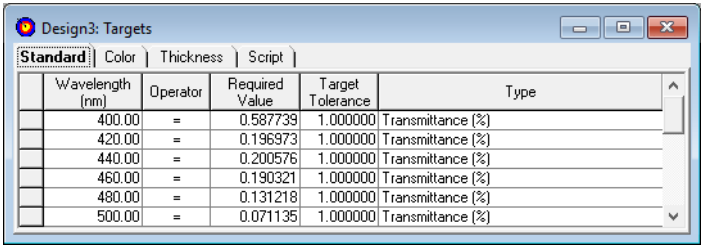
As we are importing data into the target editor, the columns of data on the clipboard must be matched to the specific columns in the target editor. To match each column, click in the header of the column, and then choose the appropriate column type in **Set Column Type**. The figure above shows the first column has been set to Wavelength.

After setting the second column to Required Value and then clicking **Next**, the data reduction screen is displayed.



Data reduction is useful when importing target data from spectrometer files. Having a large number of target points slows the optimization processes, but it is usually possible to achieve the same result with far less target points. This screen allows you to specify that a fixed number of rows are ignored between each imported data row.

The template section allows you to save the formatting information for use again later if desired.

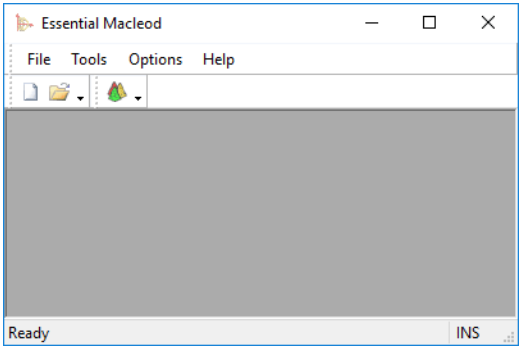


The figure above shows the Target Editor after the import was completed.

APPLICATION WINDOW

When the Essential Macleod is started, the Application Window appears. The application window is always present and forms the background to the package. The window title is always **Essential Macleod**. Below the title bar is the menu bar and toolbars. While the Essential Macleod window is blank, there are four available menus, **File**, **Tools**, **Options**, and **Help**.

During the operation of the program, the various designs, results, plots and so on appear in document windows within the application window. The document windows do not carry their own menu bar. Following standard Windows practice, they share the application window menu bar. Thus the Essential Macleod menu bar continually depends on the particular document window that is active. If it is a design window then the menu items refer to the design, if a material window, then they refer to material parameters, and so on. Clicking in a different document window to make it active automatically changes the menu bar.



This manual considers the various types of document window in turn and lists the choices available in their menus. This may seem complicated when reading the manual, but in actual use the choice is usually obvious and there is a help command, discussed shortly, that gives on-line information. This on-line information is intentionally compact. There is nothing worse than wanting a simple answer while, instead, screen after screen of detailed information pours out. The detailed information is, therefore, in this manual. You may never actually read it. We rarely read manuals either.

In accordance with standard Windows practice the menus and their items may be called either by a mouse click on the appropriate choice or by keystrokes. The keystroke for accessing any of the menus is a combination of the **<Alt>** key and the letter that is underlined in the menu title. The File menu, for example, can be accessed by pressing **<Alt> <F>** or **<Alt><f>**. The case is not important. Once the menu is activated then an individual choice of menu item may be made by pressing the underlined key by itself or with **<Alt>**. For example, once the File menu has been activated, the choice of New... may be made by pressing **<n>** or **<N>** or **<Alt><n>** or **<Alt><N>**. To close the menu without making any choice press **<Alt>**. Control menus can be accessed in different ways. For a dialog box press **<Alt><Space bar>**. For a document window press **<Alt><->**

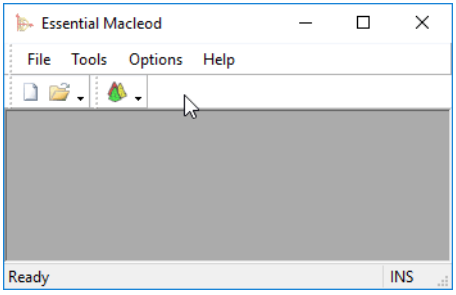
(hyphen or minus). Quick closing is **<Alt><F4>** for dialog boxes and **<Ctrl><F4>** for document windows. Clicking the close button, provided it is available, will also give quick closing. Most of these choices are obvious from the structure of the package. In dialog boxes with simple choices, use the arrow keys to change the selected option. In a document window the **<Tab>** key or the **<Enter>** key, will usually pass to the next cell for data entry.

A window can be reduced to an icon by selecting the Minimize button. Alternatively, it can be maximized by selecting the Maximize button. Both of these buttons are at the top right corner of the window. The form of the icon denotes the type of window that it represents.

The package is entirely compatible with standard Windows practice and the instructions outlined above represent only an abbreviated set of what is available. They will be assumed in everything that follows and will not be repeated.

Menu Customization

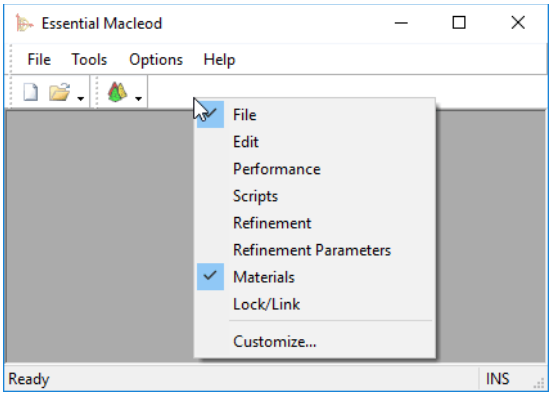
The Essential Macleod features a user customizable menu. The features of the menu system includes creating toolbars, deleting toolbars, adding icons and removing icons. The menu bar and toolbars can be docked to any edge of the Essential Macleod desktop window, or they can be placed anywhere on the screen. To move the menu bar or any tool bar, put the mouse over the grab handle at the left end of the bar and drag the bar to the desired location.



Toolbars

Add a Toolbar

Right-click in an empty part of the menu bar



and select Customize… On the Toolbars tab, click on New… and enter a name for the toolbar. The new empty toolbar will appear. To add items to the toolbar, click on the Commands tab. Drag the desired commands from the Commands list to the toolbar. If the command has an associated icon, the icon will be displayed in the toolbar; otherwise the command text will be displayed.

Delete a Toolbar

Right-click in an empty part of the menu bar and select Customize… On the Toolbars tab, select the toolbar to be deleted and click the Delete button.

Adding Commands to a Toolbar

Right-click in an empty part of the menu bar and select Customize… Click on the Commands tab. Drag the desired commands from the Commands list to a toolbar. Click Close to complete the operation.

Removing Commands from a Toolbar

Right-click in an empty part of the menu bar and select Customize… In the toolbar from which you want to delete the command, select the command and drag it off the toolbar. When the cursor changes to a cross, release the mouse button and the command will be removed from the toolbar.

Icons

Add Icon to a command

Icons can be added to any command in the menu bar. When a command is added to a toolbar, the associated icon will be displayed. If the command has no associated icon, the command text will be displayed. To add an icon, from the Options menu, select Icons and then Add Icon. Click OK to the message and then click on the menu command that will be associated with the icon to be added. Next on the Choose Icons form, click on the Browse buttons and select the file names of the icons to be used for the Normal and Disabled states. The Normal state icon is displayed when the command is available for use. The Disabled state icon is displayed when the command cannot be used (e.g. if the

clipboard is empty, pasting from the clipboard is not possible and so the disabled state icon would be displayed). The Disabled state icon is optional. If a disabled state icon is not provided, the program will generate a Disabled state icon from the Normal state icon. When each icon file has been selected, it will be displayed on the form. Click OK to complete the icon addition.

Icons may be bitmap files (*.bmp) or icon files (*.ico). The dimensions of the icons may be any size; the program will fit the image in the selected file into a 16 x 16 pixel icon. Icons can be created by an icon editor or by using a program such as Windows Paint. If the icon file is a bitmap, the top left pixel of the bitmap is assumed to be the background color of the icon. When the icon is displayed, all pixels of that color will have the actual background color in use when the program is running.

Removing an Icon from a command

Icons can be removed from a command. If the command was originally associated with an icon, this original icon can be restored to the command.

To remove an icon, from the Options menu, select Icons and then Remove Icon. Click OK to the message and then click on the menu command that is associated with the icon to be removed. The Remove Icon form will be displayed. The current icons will be shown and the original icons will be shown if available. Click Remove to remove the current icons. Click Restore to reset the icons to the original icons shown.

The Application Menu

The common commands are described below.

File Menu (Application)

New...

Selection of **New** reveals a submenu. There is a minimum of six choices, **Design**, **Material, Optical Constant**, **Table**, **Stack**, and **Substrate**. Depending on the Enhancements that are present there may also be **vStack**, **Operation**, **Machine Configuration**, **Run Sheet** and **Simulator**. Each selection produces an appropriate dialog box or document window that refers to the choice made. The selection can be made with the Mouse in the usual way or by pressing any of the arrow keys.

Design brings up a design window with the default design contained in it in the form of a table of media and layers. This is considered further below in the Design Window chapter.

Material brings up a document window headed Material that contains a blank table for entry of new optical constants and wavelength data. More details are given in the Material Window chapter.

Optical Constant brings up a new window for deriving optical constants from transmittance and reflectance data. See the section on Optical Constant Extraction for more information.

Table creates a new table after the user has indicated the number of columns required in an initial dialog box. The table is blank and the Read Only status is not set so that it can immediately be edited in the usual way. For more details, see the later section on **Edit Menu (Table)**.

Stack brings up a new document window for the design and analysis of combinations of substrates and coatings. See the Stack section for more information.

vStack brings up a new document window for the design and analysis of combinations of substrates and coatings that are not parallel. See the vStack chapter for more information.

Substrate brings up a document window headed Substrate that contains a blank table for entry of new internal transmittance and wavelength data. More details are given under the heading of Stack.

Operation creates a new Operation document. The Operation is the collection of instructions needed for a calculation by Function.

Machine Configuration creates a document where details of the machine to be used by Runsheet when generating deposition instructions.

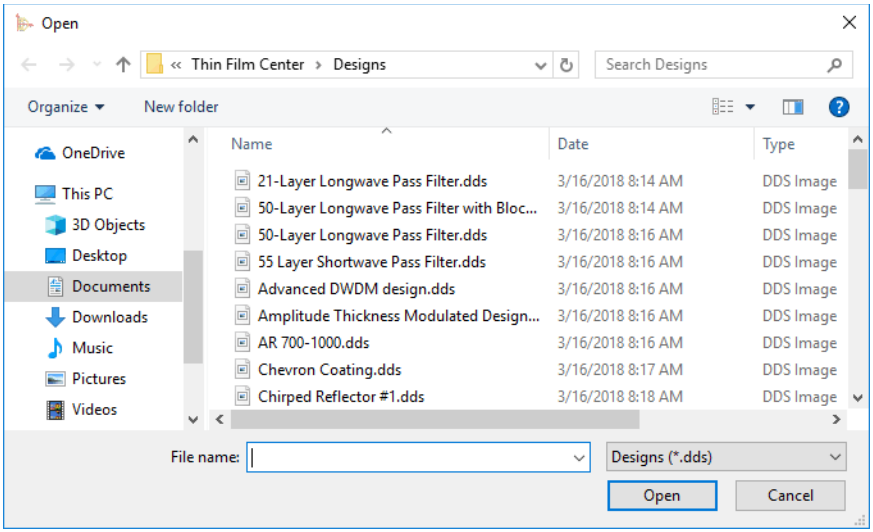
Run Sheet creates a blank run sheet where design information and a designated machine configuration will be used to generate the monitoring signals for the manufacture of the coating specified by the design.

Simulator creates a blank document for entry of the parameters such as signal noise, monitoring type, specifications of errors required for the simulation of the production of a coating specified by a given run sheet.

Report Template creates a blank document where the instructions for a report can be entered. See the Report Generator chapter for more information on the contents of a Report Template.

Open...

Open brings up a dialog box that permits any of the files that have been created by the program to be reopened. File types include designs, performance plots, performance tables, and data for optical constant extraction. These types can be selected in the drop down list at the foot of the box.



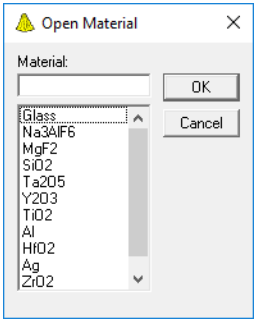
Open a Copy of...

The **Open a Copy of** command is similar to the **Open** command except that the opened item does not retain the name of the file from which it was opened. This means that the first time the item is saved, it will need to be given a file name. It is as though a new design was created and the design was copied from the existing file.

For example, use the **Open a Copy of** command to open an existing design. Now change the design in some way and then select **Save** from the **File** menu. The Save As file dialog box will appear because the design does not know the filename from which it was loaded. If the **Open** command had been used to load the design, selecting Save from the **File** menu would have saved the design back to the filename from which it was opened.

Open Material...

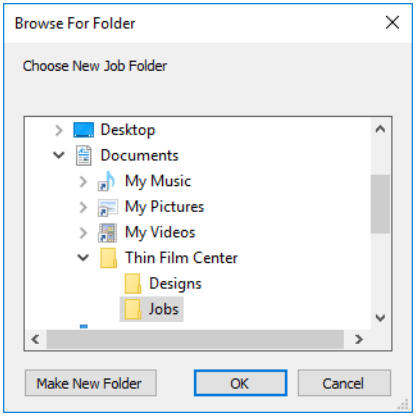
Open Material brings up a dialog box containing a list of all available materials for selection.



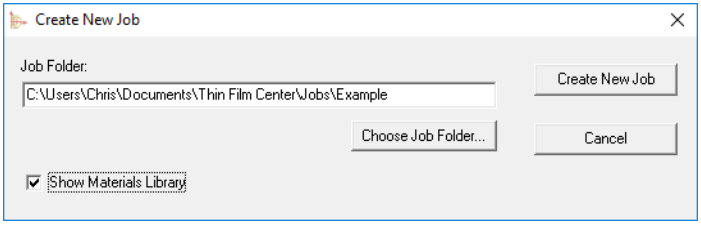
When a material is selected, a material window with the optical constants and wavelength data appears ready for editing, plotting or printing.

New Job...

New Job... creates a new Essential Macleod Job folder and populates it with a new empty materials folder, a new empty designs folder and a new references folder. Data from the standard references folder is copied to the new references folder. The first action upon selecting this command is to choose the new folder. The folder can be created anywhere in the computer, but it is recommended that the folder be created in the My Documents\Thin Film Center\Jobs folder. When the New Job command is selected, a folder chooser will appear. The folder containing the most recently created jobs folder will be selected.



To create a folder in the current selected folder, click the **Make New Folder** button. The selected folder will expand and show the newly created folder which will be named "New Folder". You can edit the name of the new folder either by selecting it and then pressing the **F2** key, or you can right-click on the folder name and click the **Rename** command. After entering the name, click the **OK** button. This will return you to the Create New Job window.



If you change your mind about the Job folder name or location, you can click the **Choose Job Folder** button to go back to the folder chooser. When the new Job folder is created, the Materials folder will be empty. You can check the **Show Materials Library** box to cause the materials library to be displayed after the job has been created. This

allows you to easily add materials from the materials library to the Job's materials database. You can also do this at any other time when the Job is open as well as import materials from other materials databases. To create the new Job folder, click the **Create New Job** button

When Create New Job has completed, the title bar of the Essential Macleod will be changed to show that a Job is open. For example, if the new Job was named "Thin Film Center", the title bar would show "Essential Macleod: Thin Film Center" The default location for saving designs etc. will be the Designs folder inside the new Job folder. The materials database will be changed to the Materials folder inside the new Job folder and the references folder will be changed to the references folder inside the new Job folder. Keeping everything in the Job folder tree makes it easy to create an archive copy of all information by making a copy of the Job folder.

Open Job...

Open Job... is used to open an existing Job. When this command is selected, a folder chooser will appear with the folder containing the last created Job folder selected. Click on the "+" symbol to the left of the selected folder to expand the list of Job folders. To open the desired Job, select the folder name and then click **OK**. The Essential Macleod will then be reset that it uses the materials database and references folder contained in the Job folder. The default location for saving designs etc. will be changed to the folder last used when the Job was previously open. The title bar of the Essential Macleod will be changed to show the name of the open Job.

Close Job

Close Job resets the Essential Macleod so that it uses the materials database and references folder that were last used when no Job was open. The default location for saving designs etc. is reset to the folder that was last used when no Job was open. The Title bar of the Essential Macleod is also changed so that it only reads "Essential Macleod" This serves as a reminder that a Job is not open.

Open Reference...

Open Reference activates a dialog box like the **Open** command but it is for reference files. Reference files contain data that is required by the program for certain calculations like the assessment of color. They are therefore treated differently from regular data files and are kept separately from them. Alteration or modification should be undertaken only with extreme caution. Data files can be converted into reference files and vice versa.

Page Setup...

Page Setup... allows the page margins to be set in a dialog box.

Printer Setup...

Printer Setup... opens a dialog box offering a choice of available printers and access to the printer options.

1

2

3

4

These menu items correspond to the most recently opened files.

More...

Opens a window showing a longer list of recently used files.

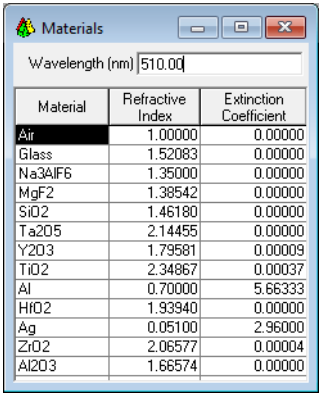
Exit

Quits and unloads the Essential Macleod. If entered or generated data are unsaved the program will display an alert box asking for instructions.

Tools Menu (Application)

Materials

This item is similar in many ways to the **Open Material...** command of the File menu. There whenever a material was selected, the dialog box closed. Here however the command brings up a materials list that is permanently visible until closed. This means that many material windows can be opened and displayed at the same time. The display of optical constants at the wavelength shown can be toggled by the **Show Optical Constants** command in the **Edit** menu for this window. To change the display wavelength, edit it in the window.



Material	Refractive Index	Extinction Coefficient
Air	1.00000	0.00000
Glass	1.52083	0.00000
Na3AlF6	1.35000	0.00000
MgF2	1.38542	0.00000
SiO2	1.46180	0.00000
Ta2O5	2.14455	0.00000
Y2O3	1.79581	0.00009
TiO2	2.34867	0.00037
Al	0.70000	5.66333
HfO2	1.93940	0.00000
Ag	0.05100	2.96000
ZrO2	2.06577	0.00004
Al2O3	1.66574	0.00000

Double-clicking any of the materials brings up a window displaying the stored optical constants. These can be edited if required, as discussed later in the manual.

Load Zemax Coating File

The Essential Macleod includes the capability of exporting coating designs to the Zemax series of lens design packages, created by Zemax LLC, to be included in

performance assessments. Zemax reads these designs together with data on materials from a coating file. The **Load Zemax Coating File** command loads the Zemax coating file into the Essential Macleod where it can then be edited.

New Zemax Coating File

The **New Zemax Coating File** command creates a new Zemax coating file in the Essential Macleod where it can then be edited.

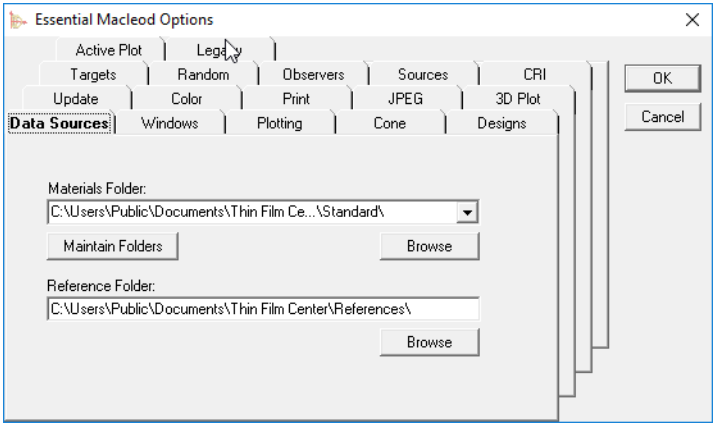
Options Menu (Application)

General...

The **Essential Macleod Options** dialog box that is activated has several features, and is divided into tabs. Selecting a tab displays a group of options.

Data Sources Tab

The upper text box contains the path and name of the current Materials Folder. This can be changed and the new folder will then be the one automatically used. A record of material databases that have been used by the package is maintained and these paths are available in a dropdown list activated by the arrow to the right of the folder name. Since a change in materials folder could have serious consequences for an existing design, it is arranged that the Materials Folder option is available only when there is no open design file.



It can be very useful to have different material files for different applications. For example, the default wavelength units in the package as provided are nm and these should be changed to microns if much infrared work is to be done. One material database can then be completely in microns and one completely in nm. It is helpful to give the materials folder a meaningful name such as IR or Visible or UV. Sometimes in the early stages of a design, nondispersive materials are used. A special folder with nondispersive materials may then be useful, called, perhaps "Non Dispersive".

Later in the manual you will find that it is very easy to create new material databases and to import materials into them. A useful way of working is to create a new materials database at the start of any new project. Only those materials that apply to the project need be imported into it. The database folder can also be used to store the design, plot and table files. Although there is no design folder in the list of options, the package will return to the same design folder each time it is loaded until another is used to store files. The data and design files are completely separated from the material files by their extensions. At the end of the project the folder will contain all the files necessary to resurrect it and it can be saved to an archive and then deleted. This technique insulates the standard materials from changes that are made only in connection with a particular project yet the special set of units that may have been used, the particular materials, the designs and so on are all preserved.

Reference files are stored in a reference folder. These are files containing data necessary for the operation of the package. In the Essential Macleod the important files in the reference folder are those containing definitions of color matching functions and of source output for the color calculations. The reference folder is also used extensively in the Function enhancement to the Essential Macleod. The Options dialog box includes a field that gives the folder where the reference files are located. Once this has been defined it will seldom be necessary to change it but the possibility does exist.

Legacy Tab

The Legacy tab provides a checkbox that permits the display of the Substrate items in the various menus so that any older substrate files can be accessed and edited.

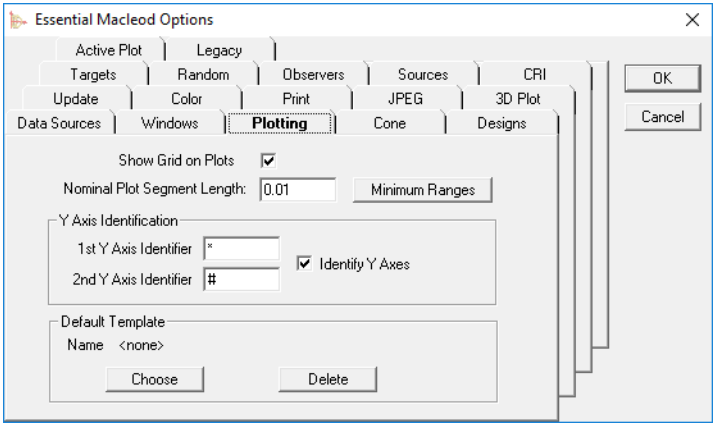
Windows Tab

When **Cascading Close** is checked any plots and tables in open windows that are associated with a given design will be closed when the design window is closed. When it is not ticked then windows will not be automatically closed.

If the **Prompt to save old Tables and Plots before closing** box is checked then the user will be asked if any plots or tables that have been changed from the version that is stored on disk should be saved before being closed.

Keep old Plots and Tables displayed is a useful option. It is very easy to accumulate many opened plots and tables. These do use up memory and should be closed as soon as they are no longer immediately needed. If this option is *not* checked then a new table or plot will simply replace any older one. If the option is checked then the new plot or table will coexist with the older.

Plotting Tab



The plots can be produced with either ticks on the axes or a complete grid. **Show Grid on Plots** decides which is to be used. Note that the plots saved by the program are stored as data rather than images. If this option is changed then all plots that are recalled from store will follow the current choice even though they may have been created with the other in force. Note that it is very easy to remove a grid from an individual plot or to restore it once removed.

Nominal Plot Segment Length has an important role in plotting. The package uses a special adaptive technique. Plots are drawn with variable spacing of successive values of the independent variable so that closely packed fringes will be reproduced without having to use a very small and inefficient interval on smoother parts of the characteristic. An algorithm calculates a starting interval from the thickness of the coating, the wavelength range and the size of the plot. During plotting, the interval is continuously varied. The nominal plot segment length is a parameter that defines the closeness of points required for the plots in general. It should rarely need to be altered. However, if you find that the kind of plot that is normally being produced is fairly flat but is taking a long time because there are too many points, then this number may be increased. If, on the other hand, the fringes are so closely packed that the program is jumping across them, then this number should be reduced. The number should be adjusted in very small increments. Halve it or double it at the most with each adjustment. It is very easy to set it so that an impossibly large number of points is required.

When the axes for plots are automatically selected, the X-axis range is scanned to estimate the total Y-axis range. This range is then used to drive the adaptive plotting algorithm. If the Y-axis range is very small, then this will force the adaptive plotting algorithm to look for very fine changes in the calculated Y values. Such plots will take a long time to calculate but they will not add any useful information. To prevent this, a minimum range can be specified. If a Y-axis is being automatically generated, then the estimated Y range is constrained to be no less than the minimum range for the performance parameter. If the Y-axis has been defined and is not automatic, the minimum range values do not apply. If you wish to modify the default minimum range

values, the **Minimum Ranges** button displays a form where you can specify the minimum range to be used for each of the available performance categories.

Plots can be generated with two Y-axes. Sometimes it may not be clear which Y-axis is used for a particular trace. Y-axis identification defines the default method by which axes are identified. If **Identify Y Axes** is checked then the titles for the Y-axes will be prefixed by the appropriate identifier and each trace will have its legend prefixed by the identifier for its Y-axis. Y-axis identification can also be manually performed in the Plot window.

A default appearance (background color, font characteristics etc.) can be specified for all plots. To set the default appearance, save a plot that has the desired appearance, then open the Plotting tab in General Options, click **Choose** and select the saved plot. To remove a previously chosen plot file, click **Delete**. Note that **Delete** does not delete the plot file.

Cone Tab

This tab provides control over the cone calculation provided by the Stack Editor. **Nominal Cone Segment Length** controls the adaptive calculation used by Cone when calculating the cone response at a particular wavelength, frequency or incident angle. It is similar to **Nominal Plot Segment Length** described above.

Bandwidth Step controls the step size when the bandwidth is non-zero.

Gaussian beams do not have a distinct cutoff where there is no irradiance. The beam intensity falls off with a Gaussian distribution. When calculating the performance of a coating illuminated with a Gaussian beam, the Essential Macleod will not calculate performance beyond a specified ratio of the Gaussian beam's semi-angle. This has the effect of truncating the edges of the beam. When the ratio is sufficiently large, the effect on the calculations will be negligible. The default value for the ratio is 2. At this limit, the intensity of the beam has fallen to 0.0003 times the on axis intensity, which should be satisfactory for most applications. To change the value of this ratio, modify the **Gaussian Calculation Scale Factor** value. Making the value larger improves the calculation results at the expense of a greater calculation time.

Designs Tab

This tab provides control over the order in which layers are displayed, the formula ordering convention and the intervals used for derivative calculations.

For the **Display Order**, there are two possible options: **Medium at Top** and **Substrate at Top**. When **Medium at Top** is selected, designs are displayed with the incident medium at the top of the list. When **Substrate at Top** is selected, designs are displayed with the substrate at the top of the list. Layers can be numbered either with the layer next to the medium numbered 1 or from the substrate.

The **Formula Order** is used to specify which end of the formula is next to the incident medium. **Medium at Left** specifies that the incident medium is at the left end of the formula string. **Medium at Right** specifies that the incident medium is at the right end of the formula string. The formula editor indicates which convention is in effect so that you do not have to remember.

Wavelength Delta Factor defines the interval used for calculating the first derivative of the optical constants. The default value has been selected to give the best performance for the majority of designs.

Optical Thickness Convention controls the display of optical thickness values. There are two options: FWOT and QWOT. When FWOT is selected, the optical thickness of a quarterwave thick layer is reported as 0.25. When QWOT is selected, the optical thickness of a quarterwave thick layer is reported as 1.

When **Use Packing Density to adjust Extinction Coefficient** is checked, the packing density value will be applied to the Extinction Coefficient data as well as the Refractive Index data. When unchecked, only Refractive Index will be modified by the Packing Density.

Update Tab

This tab provides control over the automatic checking for updates.

If automatic checking has been enabled, then, each time the Essential Macleod is started, it will first check to see if the specified number of days has elapsed since the last time a check for updates was made. If it has, then the program will connect to the Thin Film Center web site to determine if a new update is available. If there is a new update, you can choose to download and install the update now or just continue using the Essential Macleod. If you choose to download the update, the Essential Macleod will close so that the program file can be modified.

If **Automatically check for updates** is checked, then the Essential Macleod will check for updates at the specified interval. The interval is specified by entering the number of days in the box after **Check for updates every**.

Color Tab

This tab specifies the wavelength intervals to be used when calculating color parameters. The **Wavelength Interval for Performance** is used when requesting a color calculation from the menu. The **Wavelength Interval for Refinement** is used when calculating the value of a color target during refinement or synthesis. Specifying larger values increases the speed of color calculations but the accuracy is reduced.

Print Tab

This tab specifies the default header and footer to be used for printed output. The header and the footer may be multi-lined and have three sections: left, middle and right. A bar (“|”) character is used to separate the sections.

For example, the header definition:

Left|Middle Section

on more than

one line|Right

would appear as follows on printed output:

Left Middle Section Right
on more than

one line

Several symbols may be used in the header and footer. These are:

%o The type of document being printed. For example in a design this will be replaced by “Design”

%f The name of the file being printed as displayed in the title bar of the window.

%t The date when the document was printed. This will be formatted according to the date format specification at the bottom.

%d The current page number

%% Inserts the “%” character.

There are several pre-defined date formats available. These are:

Format Name	Description
General Date	Display a date and/or time. For real numbers, display a date and time, for example, 4/3/93 05:34 PM.If there is no fractional part, display only a date, for example, 4/3/93. If there is no integer part, display time only, for example, 05:34 PM. Date display is determined by your system settings.
Long Date	Display a date according to your system's long date format.
Medium Date	Display a date using the medium date format .
Short Date	Display a date using your system's short date format.
Long Time	Display a time using your system's long time format; includes hours, minutes, seconds.
Medium Time	Display time in 12-hour format using hours and minutes and the AM/PM designator.
Short Time	Display a time using the 24-hour format, for example, 17:45.

You can also design your own date format using these formatting commands:

Character	Description
(**:**)	Time separator. In some locales, other characters may be used to represent the time separator. The time separator separates hours, minutes, and seconds when time values are formatted. The actual character used as the time separator in formatted output is determined by your system settings.
(/)	Date separator. In some locales, other characters may be used to represent the date separator. The date separator separates the day, month, and year when date values are formatted. The actual character used as the date separator in formatted output is determined by your system settings.
c	Display the date as `ddddd` and display the time as `ttttt`, in that order. Display only date information if there is no fractional part to the date serial number; display only time information if there is no integer portion.
d	Display the day as a number without a leading zero (1 – 31).
dd	Display the day as a number with a leading zero (01 – 31).
ddd	Display the day as an abbreviation (Sun – Sat).

dddd	Display the day as a full name (Sunday – Saturday).
ddddd	Display the date as a complete date (including day, month, and year), formatted according to your system's short date format setting. The default short date format is `m/d/yy`.
dddddd	Display a date serial number as a complete date (including day, month, and year) formatted according to the long date setting recognized by your system. The default long date format is `mmmm dd, yyyy`.
Aaaa	The same as dddd, only it's the localized version of the string.
W	Display the day of the week as a number (1 for Sunday through 7 for Saturday).
Ww	Display the week of the year as a number (1 – 54).
M	Display the month as a number without a leading zero (1 – 12). If `m` immediately follows `h` or `hh`, the minute rather than the month is displayed.
Mm	Display the month as a number with a leading zero (01 – 12). If `m` immediately follows `h` or `hh`, the minute rather than the month is displayed.
Mmm	Display the month as an abbreviation (Jan – Dec).
Mmmm	Display the month as a full month name (January – December).
Oooo	The same as mmmm, only it's the localized version of the string.
Q	Display the quarter of the year as a number (1 – 4).
Y	Display the day of the year as a number (1 – 366).
Yy	Display the year as a 2-digit number (00 – 99).
Yyyy	Display the year as a 4-digit number (100 – 9999).
H	Display the hour as a number without leading zeros (0 – 23).
hh	Display the hour as a number with leading zeros (00 – 23).
n	Display the minute as a number without leading zeros (0 – 59).
nn	Display the minute as a number with leading zeros (00 – 59).
s	Display the second as a number without leading zeros (0 – 59).
ss	Display the second as a number with leading zeros (00 – 59).
t t t t t	Display a time as a complete time (including hour, minute, and second), formatted using the time separator defined by the time format recognized by your system. A leading zero is displayed if the leading zero option is selected and the time is before 10:00 A.M. or P.M. The default time format is `h:mm:ss`.
AM/PM	Use the 12-hour clock and display an uppercase AM with any hour before noon; display an uppercase PM with any hour between noon and 11:59 P.M.
am/pm	Use the 12-hour clock and display a lowercase AM with any hour before noon; display a lowercase PM with any hour between noon and 11:59 P.M.
A/P	Use the 12-hour clock and display an uppercase A with any hour before noon; display an uppercase P with any hour between noon and 11:59 P.M.
a/p	Use the 12-hour clock and display a lowercase A with any hour before noon; display a lowercase P with any hour between noon

	and 11:59 P.M.
AMPM	Use the 12-hour clock and display the AM string literal as defined by your system with any hour before noon; display the PM string literal as defined by your system with any hour between noon and 11:59 P.M. AMPM can be either uppercase or lowercase, but the case of the string displayed matches the string as defined by your system settings. The default format is AM/PM.

Here are some examples of user-defined date formats:

Format	**Display**
`m/d/yy`	12/7/58
`d-mmm`	7-Dec
`d-mmmm-yy`	7-December-58
`d mmmm`	7 December
`mmmm yy`	December 58
`hh:mm AM/PM`	08:50 PM
`h:mm:ss a/p`	8:50:35 p
`h:mm`	20:50
`h:mm:ss`	20:50:35
`m/d/yy h:mm`	12/7/58 20:50

In addition to the text header and and footer, graphics may also appear in the header and footer. To specify the graphic files to be used, click the **Graphics…** button at the right of the **Header** and **Footer** text boxes. A dialog will appear allowing you to choose the files containing the graphic data for the left, center and right images. At the right, the selected graphic is shown. It is resized to fit the display box and so may appear distorted. The image in the display box is only to confirm that the correct file has been chosen and does not show how the graphic will appear on the printed page.

The images are placed on the page so that in the header, the bottom of the header images are aligned with the bottom of the header and the top of the footer images are aligned with the top of the footer. If both graphics and text have been specified for the same location, then the text will overprint the graphic.

JPEG Tab

Plots created in the Essential Macleod can be exported as JPEG images. This tab provides controls for creating the JPEG data. **Quality (1 – 100)** controls the image quality. The higher the number the better quality picture will be produced, but the size of the JPEG file will also be increased. When **Gray Scale** is checked, the JPEG picture will not be in color. **Optimize Compression** improves the file size produced without reducing picture quality. When **Progressive** is checked, the JPEG will be generated so that a low quality image is displayed quickly and improves as the rest of the JPEG is loaded. This option is primarily used when the picture is to be displayed by a remote user downloading the picture file over a slow link.

3D Plot Tab

A default appearance (background color, font characteristics etc.) can be specified for all 3D plots. To set the default appearance, save a 3D plot that has the desired appearance, then open the 3D Plot tab in General Options, click **Choose** and select the

saved plot. To remove a previously chosen plot file, click **Delete**. Note that **Delete** does not delete the plot file.

Targets Tab

The targets tab contains a single option **Remove Duplicates Immediately**. When checked, duplicate targets will be removed as they are detected. For example, if the target generator adds duplicate targets, they be removed at completion of the Generate Command. If **Remove Duplicates Immediately** is not checked, then duplicate targets will not be removed, and it is the responsibility of the user to remove the duplicates. The command **Remove Duplicates** in the **Edit** menu will remove duplicate targets.

Random Tab

The random tab is used to reset the random number generator to a known state. To reset the random number generator, enter a value into the **Random Number Seed** box and click **Initialize**. Each time that you perform this action, the random generator will generate the same sequence of numbers for the same random number seed.

Observers Tab

This tab is used to specify the Observers that are available for color calculations. For more information on specifying observers, please see the Color section on page 35.

Sources Tab

This tab is used to specify the Sources that are available for color calculations. For more information on specifying sources, please see the Color section on page 35.

CRI Tab

The CRI tab is used to specify the files containing the sample spectra to be used in Color Rendering Index calculations. For more information on specifying the sample files, please see the Color section on page 35.

Active Plot Tab

The Active Plot tab is used to specify the default ranges for variables in Active Plot. The ranges are set according the type of variable. The Angle tab specifies the default range for Incident Angle. The Wavelength tab specifies the range as a multiplier of the current wavelength (reference wavelength, calculation wavelength) value. So, if the variable to be added to an active plot was reference wavelength with a current value of 510 and the multiplier for the maximum value was 2, the upper limit of the reference wavelength range will be 1020. The thickness limits are also specified as multiples of the current layer thickness. The same multipliers are used for all thickness types (optical, physical, geometric). Layer Packing Density limits are also specified as multiples of the current layer packing density values. The Link scale factors, Material Packing Densities and Taper Distances are all specified as absolute ranges.

The speed and change increments can also be controlled. When the >, <, >>, << buttons are held down, the Minimum Delay specifies the minimum time period in ms before the variable is incremented and the plot then updated. If the plot update takes longer than the Minimum Delay, then the next plot update will start immediately after the completion of the current plot update.

Each time the > and < buttons increment the value, the value is changed by Increment Proportion of the difference between the maximum and minimum values shown on the Active Plot. The default value is 0.01. That is, the value will change by 1% of the range between the minimum and maximum values.

Each time the >> and << buttons increment the value, the value is changed by Fast Increment Proportion of the difference between the maximum and minimum values shown on the Active Plot. The default value is 0.1. That is, the value will change by 10% of the range between the minimum and maximum values.

Set as Default Design

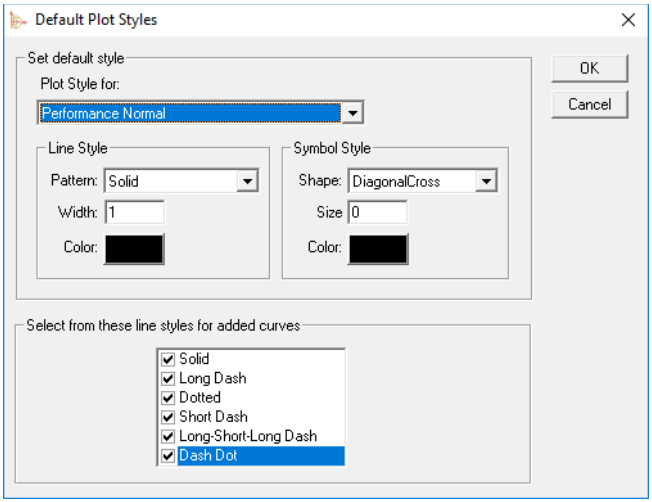
When a new design is created, a default design is used. The design that is generated by the program may not be completely suitable for all users. For example, someone who normally works in the infrared may wish to have a design with parameters suitable for the infrared rather than the visible region. It may also be that there could be a number of different standard designs that could be varied according to the particular project. This option makes it particularly easy to change from one standard design to another. It copies the active design to a default design file in the current materials database. Thus the default design will change when the database is changed.

General Units...

General units defines the units that are used when displaying information. This permits you to work in the units of your choice such as nanometres or microns, % transmittance or absolute transmittance. For more information, see the section on units in this manual (Page 32).

Chart Styles...

Chart Styles defines the styles of plotted data in the Essential Macleod. For various different types of plotted data, you can define the color, line style, and thickness of the line that will be plotted. You can also control the symbol style, color and size.



Register

This option displays the built-in registration form. Please use this form to tell us about yourself and request a site key

License

This option displays the current license and allows you to transfer a license from one computer to another. You can also enter a site key here.

Change Password

This option allows you to change the password required when transferring a license out from the computer. See the section on licensing for more information.

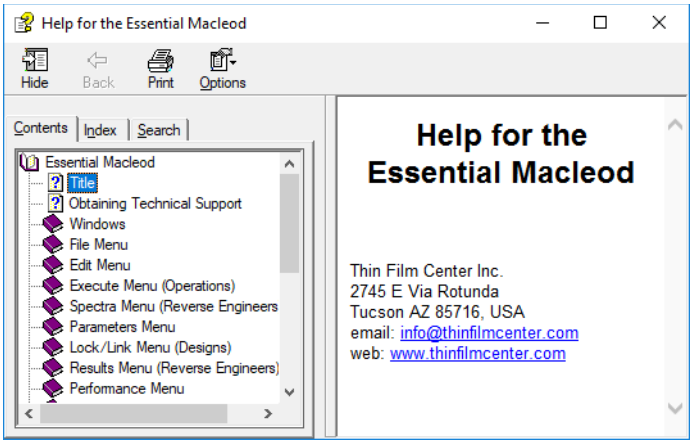
Help Menu (Application)

Contents

The **Help** menu is always available to the right of the other menus. **Contents** brings up the contents list which contains broad categories rather like the contents page of a book. The items in the contents list can be selected by clicking with the mouse in the normal way.

Search For Help On...

Selection of this menu item presents the user with the help's search dialog. After entering a word and clicking List Topics, you can click on one of the listed topics for more information.



Obtaining Technical Support...

This item lists the address, fax number and telephone number for receiving support.

About The Essential Macleod...

This gives information about the program including its version and the installed enhancements.

Check for Updates...

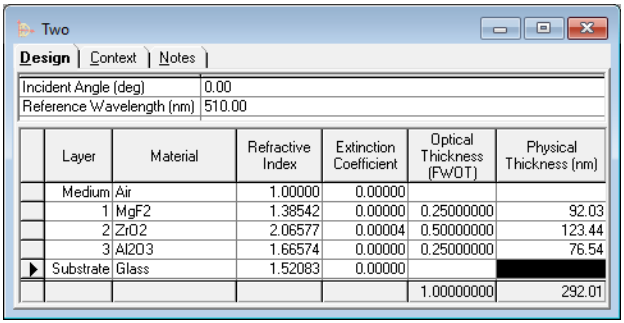
This command checks for available updates to the Essential Macleod via the Internet. If an update is available, you can then download and apply the update by clicking the Download button.

Insert/Overstrike

The bar at the foot of the Application Window displays two information boxes. The first of these will be blank at this stage. The second will contain the words **Insert** or **Overstrike**. Pressing the insert key, **<Ins>** will toggle from one to the other. These two parameters indicate the behavior of a design table when the **<Enter>** key is used to move from one cell to the next. In insert mode, pressing **<Enter>** at the end of a row will cause a new row to be inserted. In overstrike mode the cursor will move to the next existing row.

DESIGN WINDOW

An example **Design Window** is shown below. As the name suggests, it contains a coating design. The window is separated into two pages that are displayed by clicking on the tabs at the top of the window. The Design tab shows the design. The Context tab specifies the contexts available for the design. The use of context in a design is described later in this chapter in the Context section. The Notes tab provides an area for you to enter other information about the design. This design is listed following the convention: incident medium at the top of the table and substrate or emergent medium at the foot. The various layers are listed in order in between these two entries with numbers that start at 1 for the layer nearest the incident medium or substrate depending upon the design display order setting.



Above the design is listed the **Incident Angle** and the **Reference Wavelength**. To change completely either of these quantities click in the appropriate cell and type in the new value. To alter only part of the value double-click in the cell and use the arrow keys and delete keys to remove only the unwanted part and type in the corrections.

The incident angle is always referred to the incident medium. By convention the incident angle is always measured as the angle between the direction of the incident wave and the normal to the surface and is zero for normal incidence and always in the range $0° \le \vartheta \le 90°$.

The reference wavelength, λ_0, is used as a standard for optical or geometrical thicknesses. The units for the reference wavelength will be whatever units are standard in the current material database. The optical constants displayed in the tables for the various materials are also referred to the reference wavelength and it is these values that will be used by the program when it converts internally from optical thicknesses to the phase thicknesses used in the calculations.

In the thickness columns at the bottom of the Design window, the total thickness of the design is displayed. In the example given above only optical thicknesses are displayed. There are two other options, geometrical and physical thicknesses. Any of these may be displayed by using the **Display Setup** command in the **File** menu. This is detailed below.

The table may be stretched in the usual way by the mouse and it may be reduced to an icon by selecting the minimize button at the top right of the window.

The editable values, **Material** and **Layer Thickness** can be edited by choosing the cell with the mouse and then modifying the contents. A single mouse click will select the cell in such a way that subsequent entered values will completely replace the cell contents. A double-click in the cell will highlight the contents and then any entered values will be inserted at the cursor position without altering the existing values. The cursor can be moved within the cell using the arrow keys and the delete keys will delete the character next to the cursor, either before or after depending on the key. If many cells are to be altered, then **<Enter>** will move from one cell to the next and will select the contents so that any keyboard entry will replace the cell contents. **<Enter>** will then move to the next cell and the procedure can be repeated. If the cell contents cannot be edited, the optical constants for example, then keyboard entry will have no effect. If an entire table is to be entered from the keyboard then the **Insert** mode of entry may be useful. This will be indicated by the word **Insert** in the status bar at the foot of the Essential Macleod Window. In Insert mode when the current cell is at the end of a row and **<Enter>** is pressed then a new row will be inserted in the table. If new rows are not to be generated then the mode should be changed to **Overstrike** by pressing **<Ins>**. Then if the current cell is at the end of a row **<Enter>** will cause the cursor to pass to the cell at the start of the next existing row and no new rows will be created.

The following sections describe the commands that are available for the design window.

File Menu (Design)

New...

This is the same command as **New...** under the **File** menu for the application window. It brings up a submenu that includes the choice of **Design**, **Material** and **Table**. These imply a new design, a new material or a table. Other choices may be available depending upon the installed enhancements.

Open...

This command presents the user with the usual dialog box showing a file list for opening. The file type can be changed so that designs or plots, or tables can be presented.

Open a Copy of...

This command presents the user with the usual dialog box showing a file list for opening. The file type can be changed so that designs or plots, or tables can be presented.

Open Material...

This command presents a list of the materials in the current materials database for opening. Note that another way of opening materials data files is provided by the **Materials** command in the **Tools** menu.

Open Reference...

This command presents a list of the reference files in the current reference folder for opening.

Close

Close closes the active window. If the information in the window has not been saved since the most recent changes then an alert box will offer the choice of saving, discarding or aborting the close. If the close operation concerns a design then if **Cascading Close** has been selected as a standing option, all windows that present results connected with the design will also be closed.

Save

Save saves the active window contents in the file from which it was either read or last saved.

Save As...

Save As... permits the active window contents to be saved in a new file or an existing file that is not necessarily the file from which the data was read or where it was already saved. A dialog box asking for a file name is presented and either a new name can be entered or an existing one selected from the list. Note that the appropriate extension will be added to the file name quite automatically. It is not necessary to type it in. Further, once the name has been correctly entered then pressing the **<Enter>** key is sufficient to initiate the save operation.

Save All

This command is most useful when a number of windows are open and all have to be closed. If they have not been saved since the last alteration then the usual alert box will be presented for each in turn.

Export

The Essential Macleod can export designs for use in Zemax, FRED, LinkSIM and CODE V.

The submenu **Add to Zemax File** converts designs to Zemax format for use with the Zemax lens design program. See page 40 for more information on this command.

The Command **FRED File** is used to export the design for use with the FRED optical modeling program. See page 44 for more information on this command.

The command **LinkSIM Filter File** is used to export the design for use with the LinkSIM simulation program. See page 43 for more information on this command.

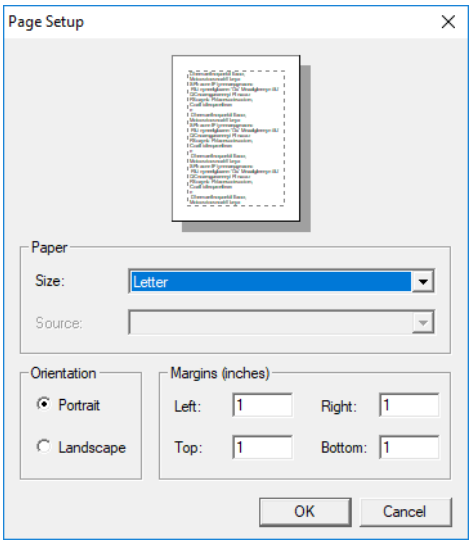
The command **CODE V Sequence File** is used to create a sequence file for CODE V. See page 43 for more information on this command.

The command **Spektrum Design...** is used to create a file that can be read by the Spektrum program from Laser Zentrum Hannover. After selecting the command, the only information required is the file where the data will be stored is entered.

There may also be entries for Monitorlink enhancements that export the design formatted for the deposition controller being used. For more information, see the Monitorlink chapters.

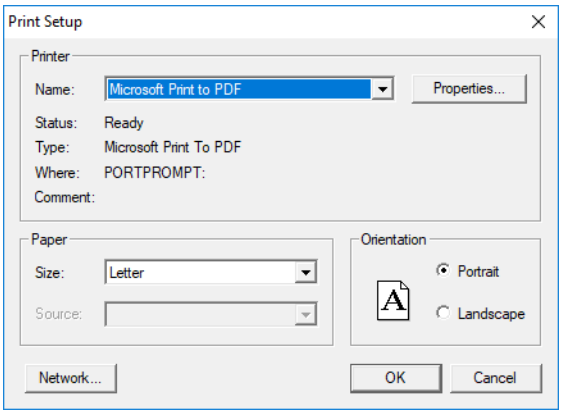
Page Setup...

Page Setup... applies to the printed page not the screen. (The screen equivalent is the **Display Setup >** command below.) The dialog box shows the columns that will be printed when the **Print** command is chosen. Access to the margin settings is given.



Printer Setup...

A typical example of the dialog box is shown below. A printer can be chosen and the paper orientation changed. The **Options...** button gives access to the parameters that apply to the active printer.



Print

Print prints the design table to the current Windows printer. The format of the printed output is controlled by the report template DefaultDesign.rpx stored in the current materials folder. See the Report Generator chapter for more information on the formats of the report template.

Print Preview

This command shows you, in a separate window, how the design would appear if it were printed out.

Print Report

Print Report prints the design table to the current Windows printer formated according to the selected report template. After selecting this command a file chooser will appear that allows you to select the report template to be used, See the Report Generator chapter for more information on the formats of the report template.

Preview Report

This command shows you, in a separate window, how the design would appear if were printed using the selected report template.

Display Setup >

The default display has a limited number of columns that represent the information that is required for most applications. These are shown in the design table reproduced above. Layers, however, may have a packing density other than unity assigned to them and they may be either locked or linked in the refinement processes. (See the note on packing density in the earlier section on the Structure of the Essential Macleod). There are several ways in which packing density may be altered. For straightforward manual entry the packing density column in the design display may be edited in the same way as any of the other columns. To reveal the column so that the entries may be changed, the item simply has to be checked in the sub-menu that is opened by this command.

Locking and linking are described in detail below. Although they can be edited by activating the appropriate columns there are other ways involving the **Link/Lock** menu that will usually be easier.

When layers have a non-unity packing density, a material can be specified for the void and the packing density of the material within the void can also be specified. The columns used are Void Material and Void Density. They may be displayed by selecting the appropriate sub-menu items.

Layers may also have an inhomogeneity factor. This specifies a change in refractive index through the layer. This is described in the Inhomogeneity Factor section below.

During refinement, minimum and maximum limits can be placed on the thickness of each layer. Selecting the Minimum Physical Thickness and Maximum Physical Thickness items displays the columns for defining the limits in terms of physical thickness. Selecting the Minimum Optical Thickness and Maximum Optical Thickness items displays the optical thickness limit columns. For Simplex refinement, limits can also be placed on the packing density of each layer. Selecting the Minimum Packing

Density and Maximum Packing Density items displays the packing density limit columns.

The sub-menu will remain open until either the Close item is selected or the mouse is clicked outside the sub-menu.

1

2

3

4

The last four files that have been opened or saved by the program are displayed here. Any of these files can be opened simply by selecting the file. It is not necessary to use the regular **Open...** command.

More...

More opens a dialog showing a longer list of recently opened files. Double-click on a file in this list to open it. You can also change the displayed order of the files and remove files from the list. Selecting a file and clicking **Move Up** moves the filename towards the top of the list. Similarly, clicking **Move Down** moves the filename towards the bottom of the list. Clicking **Remove** will remove the filename from the list.

Exit

Exit unloads the Essential Macleod inviting first the saving of any open files that have been altered since the last save.

Edit Menu (Design)

The **Edit** menu helps in the editing of designs by cutting layers, copying them, copying parts of designs and so on. It also permits the entry of a design from a formula and the changing of the way in which layers are displayed. Some parameters that are used in refinement can also be set or canceled from this menu. Note particularly that the commands in this menu cannot be undone. Save the design before major editing!

Undo and Redo

Changes in the structure of the design are remembered and can be undone and/or redone by these commands. All changes since the design was opened are remembered but are lost when the design is closed.

Cut Layers

Layers that are selected in an active design window are cut out and placed on the clipboard. From there they can be pasted into another design, into a different part of the same design, or pasted into a text document for editing by a word processor. In fact the clipboard is the normal vehicle for importing or exporting data to or from the program.

A word about selecting layers is necessary. To select a range of layers, first select one of the layers at the extreme end of the range. Then move the cursor to the selection box for the layer at the other end of the range and press **<Shift>** this time while clicking in the

box for the second time. The entire range of layers between the two limits will now be selected. To deselect a layer or range of layers, first select one of the boxes belonging to one of the selected layers. Then click once in the box and all layers will be deselected. It is sometimes useful to be able to select layers that are not contiguous. To select an additional layer that is separated from the others press **<Ctrl>** while clicking in the selection box.

Copy Design

This command will copy an entire design and place it on the clipboard.

Copy Layers

This command is similar to the **Cut Layers** command except that the layers are not removed but only copied.

Copy Thicknesses

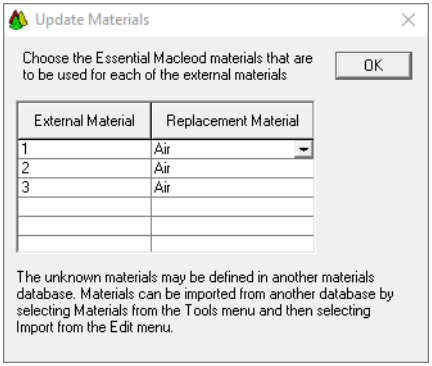
This command copies the entire set of layer thicknesses from the design and places them on the clipboard. The thickness convention (optical, geometric, physical) is specified by selecting the convention from the sub-menu. The reason for this is to make systematic alteration of the thicknesses possible. It may be required, for example, to change the thicknesses gradually from one end of the design to the other to simulate, say, a gradual change in the pattern of distribution. This command extracts just the thicknesses and a companion command, **Paste Thicknesses** will return them. *Note that noncontiguous layers can be selected for copying and pasting. Press* **<Ctrl>** *when clicking in the selection box to select a noncontiguous layer.*

Paste Design

This command pastes a design from the clipboard into a selected design window or selected design icon. The design may have been copied from another design file. The format of the design on the clipboard will then be a private format that exactly corresponds to the new design window and the pasting operation will proceed automatically and accurately. The pasted design will replace completely the existing design.

The **Paste Design** command may be used, however, to paste a design imported from elsewhere. A typical example is a design in text form in a text processor. The design should be in the form of tabulated data. Each row in the table corresponds to a layer in the design and each column in the table corresponds to a property of a layer such as thickness. The character used for delimiting columns is not important, it can be specified when the design data is imported. When the **Paste Design** command is activated the data import tool is displayed. Using this tool you specify the layout of the table by choosing the column delimiter and identifying the data contained in each column. At the end of this process, the data will be imported into the design editor. The section Importing Data on page 44 describes the use of the data import tool. After the table data has been imported, the materials used in the table need to be identified. A second dialog box will appear. In the example below, the copied design used materials numbered 1 and 2. They must now be translated into materials in the current database. The converted names may be typed in or the arrow at the end of the cell used to activate a drop down list for selection. Should the materials in the database not correspond to what is required the materials should be converted into different arbitrary, but existing, materials. This way the design can be

imported. It is easy to change the materials later to those in a new database or to ones that have been added to the current database. See the **Edit Materials...** command below.



Paste Layers

This command pastes layers from the clipboard into an active design window. The layers are pasted into the design immediately before whichever layer has been selected, that is, has an active cell.

Paste Thicknesses

This command permits manipulations of layer thicknesses outside the package and adds flexibility to the design editor. It pastes a set of thicknesses from the clipboard into a design. The convention of the pasted thicknesses (optical, geometric, physical) is specified by selecting the convention from the sub-menu.

Should the number of layer thicknesses to be pasted not correspond exactly with the number of layers in the design, then a dialog box will ask whether the updating process should continue. If continued then the thicknesses will be applied, in order, to the layers starting with layer 1 and stop when either the number of entries on the clipboard or the final layer of the design is reached.

The flexibility of the command can be increased if it is used along with other Edit Menu commands such as **Copy Layers** and **Paste Layers**. For example, create a temporary design as a holding area and paste thicknesses into it. Then use **Copy Layers** and **Paste Layers** to place the layers anywhere in the actual design.

Note that no information on the thickness convention is carried with the thickness values on the clipboard. Such information is, of course, included when **Copy Layers** and **Paste Layers** are used.

The format of the thicknesses on the clipboard must be correct and especially important is that there should be no final formatting character such as an end of line or paragraph marker. When copying them to the clipboard it is best to avoid including the line terminator for the final thickness. Place the cursor immediately after the last digit of the final thickness and drag to the start of the column to select it. If, when attempting to paste the thicknesses, a message: "The data on the clipboard are not suitable for updating the thicknesses of the layers" is displayed, it will usually mean that the copying to the

clipboard has included some extra control characters and another attempt at selecting and copying will usually succeed. Note that some word processors do not place the data on the clipboard in a compatible format. If difficulty with such processors or other systems is experienced then an intermediate step of pasting the contents into either Notepad or Wordpad and then recopying them to the clipboard will usually strip off the offending characters. Sometimes too, the command **Paste Design** will function when **Paste Thicknesses** fails. Since **Paste Design** with only one column of results will lose any material information that is present in the existing file, it is better to paste the layers first into a new, temporary design and then to use the copy commands to move them to the correct place.

Insert Layers...

A dialog box asks for the number of layers required. They are then inserted in the design immediately before the currently selected layer. The thickness of the inserted layers is zero and the material is nominal, usually Na3AlF6. Once the layers have been inserted they should be edited as required. Note that insertion of a small number of layers is most easily carried out by first making sure that the editor is in insert mode shown by **Insert** on the bar at the foot of the application window. If **Overstrike** is shown then press **<Ins>** once to change it. Click anywhere in the layer *before* the place where the new layer is to be inserted. Press **<Enter>** repeatedly until the active cell becomes the last one in the row. The next press of **<Enter>** will create a new layer in the correct place.

Delete Layers...

This deletes a specified number of layers starting with the currently selected layer and working towards the substrate.

Reverse Layers

This could be the most important menu item in the package. The convention throughout the package for the order of layers in a design is is set by the user. In the default mode layer 1 is the layer next to the incident medium. In the **Formula** the layers run from incident medium at the left to substrate at the right (this is the same convention usually used in simple optical systems) unless this too has been specified. There is, no universal agreement on either direction or numbering arrangement. The difficulties are compounded because the convention is not always clearly stated and it is only when a design is calculated that it becomes obvious that the order is incorrect. It is quite possible, therefore, that a laboriously entered design might have been placed in the tables in reversed order. This menu item affords a simple remedy. **Reverse Layers** immediately reverses the order of the layers without altering the position of substrate and incident medium. If a contiguous set of layers is selected, then Reverse Layers will modify only those layers.

Reverse Design

Reverse Design reverses the order of the layers, swaps the substrate and incident medium and changes the incident angle

Formula

Formula permits designs to be set up or edited using shorthand notation and handles the definition of the symbols used. The shorthand notation is a particularly convenient

way to enter layer data. The design is represented in terms of basic layers, of differing materials, which are represented by symbols such as H, L, A, B, c, d etc. The **Formula** command does not differentiate between upper and lower case characters. The basic layer definition is given by the material, the layer thickness (either physical or optical), the packing density, lock and link specifications for refinement, the void material and the void material density, inhomogeneity factor, minimum and maximum physical thickness limits for refinement. Layer thicknesses other than the basic thickness are represented by multiples of the basic thickness, as in, for example, 2.5H or 0.4L (representing 2.5*0.25 = 0.625 full waves and 0.4*0.25 = 0.1 full waves respectively, if the basic thickness were 0.25). The symbols can be combined into a formula using a simple sequence as in A2LB2LA or repeated sequences can be included in brackets with an exponent or replication factor, e.g.

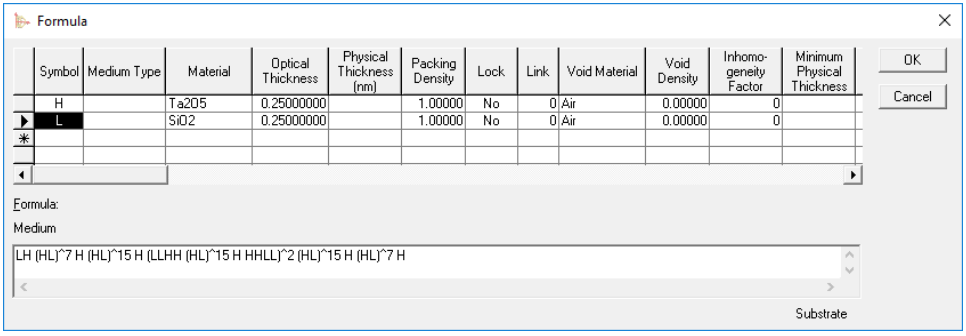
(HL)^6 3.4H2.1L

or

((H1.2L2B)^2 HL)^3 (LBH)^2

Note the space between the exponent and what follows. If it is omitted the program will reject the formula. Multiplying factors outside brackets can be used. They will be applied to all layers inside the brackets. For example **2.3(HL)^3** would be interpreted as **(2.3H 2.3L)^3** and **1.1(A 2.3(HL))** would be interpreted as **1.1A 2.53H 2.53L**. The incident medium may either be at the left end or the right end of the formula and depends upon the setting specified in the **Design** tab of the **General** command in the **Options** menu. There are some keyboards where the caret symbol ^ is not readily available (German keyboards for example), and the asterisk, *, can be used as an alternative. Brackets can be nested within brackets with almost no limit on depth.

Selection of the option brings up a dialog box for the entry of the basic layer definitions. Any existing symbols are retained and presented first in the list. To delete an entry, select the symbol and press **<Del>**. Once the symbols have been defined, the formula can be entered in the Formula box. For clarity, the formula may be entered on more than one line to show, for example, structure in the design. Arrow keys or the scroll bars can be used to scroll to either end of the formula if it is too large to be displayed completely in the box. Select the OK button to replace the current design with the design given by the formula. Should there be an error in the syntax of the formula it will be flagged at this stage with an indication of the specific error. A corrected formula can then be entered.



The text box in which the formula is entered accepts the usual copy, cut and paste commands. These can also be used to transfer part or all of a formula to a different design.

Note that the interpretation of the entered formula does take account of the match angle. Match angle is described below. If **Formula…** ever appears to be operating in a curious way, check the match angle option to make sure it has not been set inadvertently to an incorrect angle.

Generate Rugate...

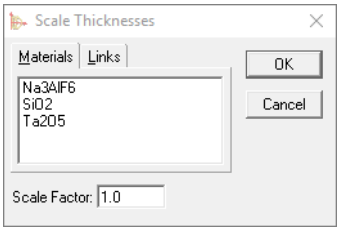
This command allows you to easily generate models of rugate coatings. The continuously varying refractive index of a rugate coating is modeled by a sufficiently large number of layers with a discretely varying refractive index. The variation in refractive index is achieved by varying the packing density of each layer. The Generate Rugate command allows you to easily specify the index variation and control the number of layers that are used to model the rugate structure. See the section “Modeling Rugate a Coating” below (page 105) for more information on modeling rugate coatings.

Generate Design...

This command allows you to generate more complex designs than can be produced by the Formula command. For example, chirped reflector models may be produced using this command. See the section “Generating Complex Designs” below for more information.

Scale Thicknesses...

Occasionally layers of a particular material or that have the same link number should have their thicknesses changed in the same way. This would happen most commonly in reverse engineering when investigating the effects of lack of uniformity but there are also times when slight adjustments must be made to the width of a pass or stop band. It is also sometimes necessary to retain the value of a particular reference wavelength but to change all layer thicknesses in the same ratio so that the characteristic is shifted but otherwise essentially unchanged. The **Scale Thicknesses...** command makes all this particularly easy.



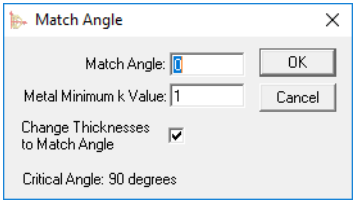
The dialog box that appears will show either the materials that are used in the design, or the links that are used. Click on the Materials tab to show the materials or click on the Links tab to show the links used. The scale factor that is entered applies to all selected materials when the OK button is clicked and the Materials list is visible. If the Links list is visible, then the scale factor is applied to the layers with the selected link numbers.

Match Angle...

All the parameters listed in the design table and the output of the **Formula...** command assume normal incidence. But whenever a multilayer is tilted, the phase thicknesses of the layers vary with the cosine of the angle of incidence in the layer and this effect is responsible for the shift in the characteristic towards shorter wavelengths. A coating that is actually to be used at oblique incidence should have the thicknesses of the layers adjusted accordingly. The lower the refractive index of the material the greater is the necessary adjustment. Layers that have been corrected for a particular angle of incidence are said to be matched for that angle. The **Match Angle...** menu item makes the calculations and adjustments automatically.

Metals and dielectrics behave differently, although the same fundamental principles are involved. High performance metals, because they have very low refractive index and high extinction coefficient, do not exhibit the appreciable shift of dielectrics and should not be corrected. In order to classify materials either as metals or dielectrics an arbitrary dividing line uses a preset level of extinction coefficient. This level is normally unity but can be changed by the user. If the actual extinction coefficient is higher than the limit, then the material is classed as a metal and no correction is made. If the extinction coefficient is lower, then the dielectric correction is implemented.

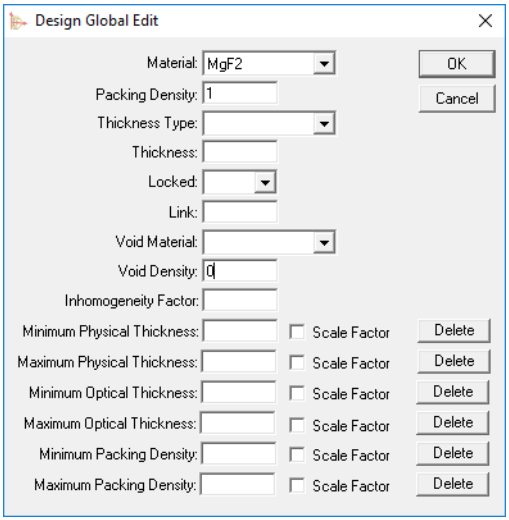
Note that the correction changes the normal incidence thickness to correct the behavior at oblique. The design table values still apply to normal incidence. Any pasting operation ignores the match angle. **Formula...**, however, does recognize the match angle and does correct layers accordingly. If **Formula…** ever appears to be operating in a curious way, check the match angle option to make sure it has not been set to an incorrect angle.



Changing the match angle is straightforward. The new value is entered in the dialog box. The operation first returns the layers to normal incidence and then applies the new angle. The current match angle can always be found by selecting the match angle menu item and looking at the displayed value.

Global Edit...

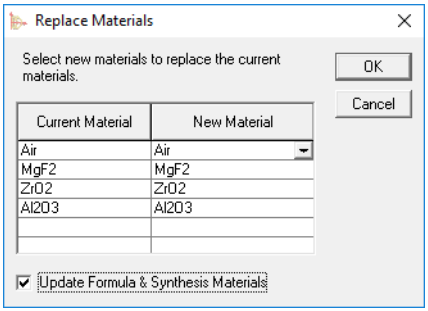
This command changes either all layers in the design or selected layers only, if at least one layer has been selected to values entered on the Global Edit form.



If a value is entered into one of the fields, then the layers will be updated with the new value. If the field is left blank, then the value held in the layer will be not altered. For the layer parameter limits fields, there is the additional option of specifying that the entered value is a scale factor. When Scale Factor is checked, the value entered into the appropriate limit cell in the Design will be the product of the scale factor and the corresponding layer parameter. For example, if a Minimum Physical Layer Thickness of 0.95 is entered and Scale Factor is checked, the minimum physical thickness of each layer will be set to 0.95 * the layer's physical thickness. This makes it easy, for example, to set thickness limits as a percentage of the current layer thickness. Click **OK** to cause any changes to be made. Clicking **Cancel** causes the edit operation to be aborted. In the example the material of the layers will be changed to MgF2, the packing density will be set to unity and the void density will be set to zero.

Edit Materials...

Edit materials offers a simple way of changing the materials in a design. The user simply inserts the translation in a dialog box. When **Update Formula & Synthesis Materials** is checked, the material names in the formula and synthesis materials list will be changed to the new materials. If it is not checked, only the materials in the design will be changed.



Create Design

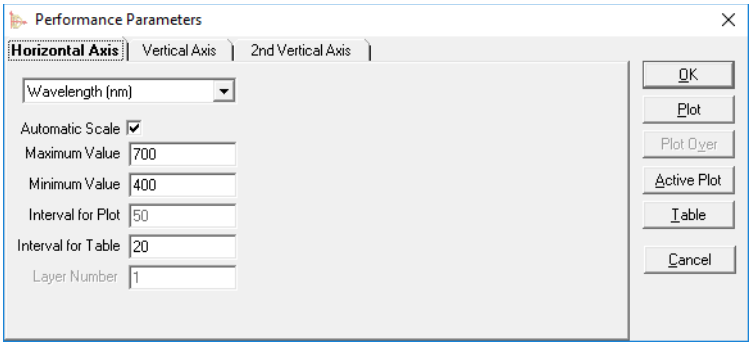
Create Design creates a new design consisting of only thin film layers from the current design. A design may contain thick as well as thin layers. Some performance calculations such as phase and analysis calculations cannot be performed when a design contains thick layers. This command takes a set of contiguous thin film layers in the design and creates a new design using those layers. The incident medium of the new design is set to be the same material as the thick layer at the incident medium end of the contiguous thin layer set (or the incident medium if there is not a thick layer). The substrate of the new design is set to be the same material as the thick layer at the substrate end of the contiguous thin layer set (or the substrate is there is not a thick layer).

To create the new design, select any thin layer in the contiguous layer set and then click Create Design.

Parameters Menu (Design)

Performance...

The performance parameters consist mainly of the choice of the quantities and scales of the axes in the performance plots that are to be produced. One or two Y axes may be defined. Tables will use the same parameters and range of independent variable and just the independent variable interval for the tables needs to be separately specified. The content of the table will be defined by the performance requested in the Vertical Axis tab. A typical dialog box for entry of the performance parameters is shown below and is reasonably self-explanatory. Items not available for the particular choice of dependent quantity are gray and cannot be accessed. The parameters described here only apply to designs that consist solely of thin layers. When a design includes one or more thick layers, a modified performance parameters dialog is shown. This dialog excludes the phase related options, but adds cone and bandwidth calculation options. See the Coherence, Cone and Bandwidth section of the Essential Macleod Structure chapter for more information.



The package computes the response, the dependent variable, in terms of a variable parameter, the independent variable. Except for a very few special cases, throughout the package the vertical axis in the plots corresponds to the dependent variable while the horizontal axis corresponds to the independent variable.

The dependent variable, the performance, may be chosen from the scrolling list under Vertical Axis. This list comprises

Transmittance Magnitude (%)
Reflectance Magnitude (%)
Transmittance Phase (deg)
Reflectance Phase (deg)
Back Reflectance Phase (deg)
Back Reflectance (%)
Density
log(Transmittance) (dB)
log(Reflectance) (dB)
Absorptance (%)
Reflectance GD (fs)
Reflectance GDD (fs^2)
Reflectance TOD (fs^3)
Transmittance GD (fs)
Transmittance GDD (fs^2)
Transmittance TOD (fs^3)
Transmittance Delta (deg)
Transmittance Psi (deg)
Reflectance Delta (deg)
Reflectance Psi (deg)
Transmittance CDC (fs/nm)
Reflectance CDC (fs/nm)
Transmittance PM
Reflectance PM

The phase parameters may be calculated in two ways depending on whether **Unwrap Phase** is checked or not. If Unwrap Phase is checked, the phase values will not be constrained to a principal angle range but allowed to continuously increase (or decrease) beyond the principal angle limits. If Unwrap Phase is not checked, the phase values will

be constrained to the principal angle range. For example if the Phase limits have been set to –180 to +180 degrees and Unwrap Phase is checked, the resultant value of a phase calculated as –179 degrees where the previous value is +179 degrees will be 181 degrees. This form of phase plot will show the phase characteristic as a continuous line, whereas the wrapped form will have discontinuities where the phase crosses the principal angle boundaries.

GD indicates Group Delay, GDD, Group Delay Dispersion and TOD is Third Order Dispersion. These quantities are important in components for ultrafast applications and are directly related to the derivatives of phase shift with respect to the angular frequency of the light.

CDC indicates Chromatic Dispersion Coefficient. This quantity is similar to Group Delay Dispersion in that it indicates pulse spreading. It is more commonly used in the communications field.

PM indicates Polarization Maintenance. This parameter calculates how much the coating changes the polarization state of the incident beam. Polarization maintenance is typically measured by placing a polarizer in the incident beam aligned at 45° to the p and s-directions, and an analyzer in the emergent beam. The analyzer is first aligned parallel to the input polarization to give the signal irradiance and then orthogonal to it to give the leakage irradiance. The irradiance in the signal orientation divided by the sum of the irradiances, expressed as a percentage, is the measure of polarization maintenance.

Derivatives with respect to wavelength of those quantities that are not already derivatives can be specified by entering the appropriate derivative order in the derivative field. For example, the first derivative can be specified by entering unity in the box. Please note the comments under Derivatives in the Essential Macleod earlier in this manual.

The independent variable is specified in a similar scrolling list under Horizontal Axis. There are essentially four different types of independent variable, wavelength, frequency, incident angle and layer thickness. The actual terms displayed in the scrolling list follow the names that have been entered in the General Units dialog box.

The thickness of a chosen layer may be used as the independent variable. This is immediately applicable to the case of an etalon with variable spacer layer but there are often cases where the sensitivity of performance to variations in the thickness of a particular layer is in question.

Plots and tables using the current values of the parameters can always be initiated from the **Performance** menu. However, the **Performance Parameters** dialog box gives immediate access to either plots or tables without the necessity of returning to the menu. If the OK button is chosen then the only immediate action taken will be to change the current values of the parameters to those entered so that they will then be used by the plot and table commands in the **Performance** menu. They will not be stored permanently in the design file until it is actually saved.

To aid in identifying traces on a plot, plot parameters may be automatically added to the plot legend by checking the **Add to Label** box next to each parameter. If the **Plot Targets** box is checked, then the targets will be added to the plot if the performance type of the targets matches the performance specification of the plot.

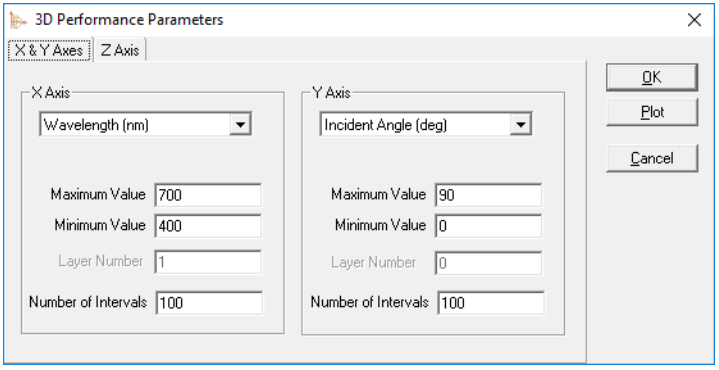
Refinement

Choosing **Refinement** in the **Parameters** menu brings up a submenu that gives access to the various parameters that must be set before effective refinement and synthesis is possible. There are two aspects of the parameters that need definition. First there are the specifications of the desired performance levels. These are called **Targets** and they are common to all the various techniques. Then there are various attributes that must be set correctly for the particular technique that is to be used. The principal technique in the Essential Macleod is Optimac, a powerful synthesis method that can also carry out refinement. Five further refinement techniques are Nonlinear Simplex, called nonlinear to distinguish it from a similarly named but different technique used in the solution of linear equations, a statistical method known as Simulated Annealing, two derivative methods: Conjugate Gradient and Quasi-Newton and an evolutionary method: Differential Evolution. Additionally, the Needle synthesis method is available for generating designs.

Refinement and synthesis are discussed in a later dedicated section.

3D Performance...

The 3D performance parameters consist mainly of the choice of the quantities and scales of the axes in the 3D performance plots that are to be produced. A typical dialog box for entry of the 3D performance parameters is shown below and is reasonably self-explanatory. Items not available for the particular choice of dependent quantity are gray and cannot be accessed.



The package computes the response, the dependent variable, in terms of two variable parameters, x and y.

The dependent variable, the performance, may be chosen from the scrolling list under Z Axis. This list is the same as in the Vertical Axis in the Performance Parameters dialog.

The independent variables are specified in similar scrolling lists under X & Y Axes. There are essentially four different types of independent variable, wavelength, frequency, incident angle and layer thickness. The actual terms displayed in the scrolling lists follow the names that have been entered in the General Units dialog box.

The thickness of a chosen layer may be used as the independent variable. This is immediately applicable to the case of an etalon with variable spacer layer but there are

often cases where the sensitivity of performance to variations in the thickness of a particular layer are in question.

The surface computed in a 3D plot is calculated at a fixed number of equally spaced points in the x and y directions. The **Number of Intervals** parameter specifies then number of points calculated.

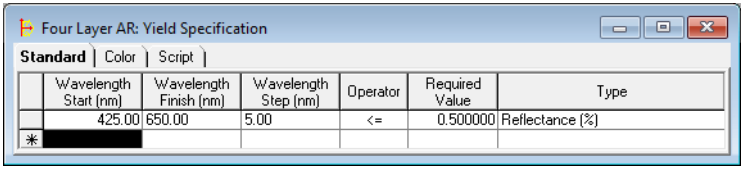
3D Plots using the current values of the parameters can always be initiated from the **Performance** menu. However, the **3D Performance Parameters** dialog box gives immediate access to a plot without the necessity of returning to the menu. If the OK button is chosen then the only immediate action taken will be to change the current values of the parameters to those entered so that they will then be used by the 3D plot command in the **Performance** menu. They will not be stored permanently in the design file until it is actually saved.

Yield Specification...

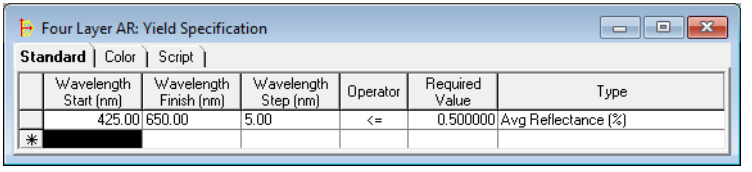
A Yield Specification is used in conjunction with the Errors tool to calculate the proportion of perturbed designs generated by the Errors tool that meet the Yield Specification. This proportion is an estimate of the number of manufacturing runs that will result in acceptable parts.

The Yield Specification is very similar to the Targets used by refinement except that for Standard performance parameters a wavelength range is specified rather than individual wavelengths. Additionally, the operators available are >= and <=. This allows the creation of a test where a performance value must lie within a certain range where one row provides the upper bound and another row provides the lower bound. For a perturbed design to be acceptable, all entries in the Yield Specification must be satisfied.

For example, the Yield Specification below requires that reflectance be less than 0.5% over the wavelength range 425 to 650 nm. The reflectance is tested at 5 nm intervals throughout that range.



If, for example, the requirement is that the average reflectance be less than 0.5%, this is entered using the Avg Reflectance type in the Yield specification.



Performance Menu (Design)

The **Performance** menu controls the calculation of performance figures by the package. Access to the menu items is possible only when a design window is active and the calculation initiated by the choice of one of the items will refer to the design in the active window. There are two principal ways in which the results of a calculation may be presented. They may be plotted or tabulated and either may be chosen from the menu. Another aspect of performance of a design is its susceptibility to errors, also available from this menu.

Plot

Plot initiates the plotting of performance in a plot window. The aspects of performance and the range over which they are to be plotted have already been chosen under the item **Performance** in the **Parameters** menu.

The Plot window is now the active one and so the menu bar changes to reflect that. The principal changes are that the **Performance** and **Parameters** menus disappear and the choices under the others are limited.

Many aspects of the plot can be modified. The section on the Plot Window later in this manual describes how plots may be modified. Note that the performance data do not change when the plot parameters are altered. If a change is made to the wavelength region outside the range of the original calculations then the altered plot will simply be blank over the new part of the region. To extend the wavelength region outside the original limits it is necessary to return to the design window and select **Performance** in the **Parameters** menu. The dependent variable is not limited in this way.

Plot Over

Plot Over permits the plotting of a second curve to be made over a first. The first curve must have been made using the current design. Once the first curve has been produced, then an adjustment to the design or a change in the calculation parameters, such as angle of incidence, may be made and then the performance of the new arrangement plotted over the first.

Plot Over will be grayed out if the design file is changed. To plot the results of a different design over those of a first, the **Add** command in the **File** menu should be used. Plot the results of the first design. Save the plot as a plot file using the **Save As...** command (the short cut key **<F12>** is the quickest and most convenient way of doing this). Change to the alternative design. Plot the results. While the plot window is active, choose **Add Line...** from the **File** menu (**<Alt><f>** followed by **<d>**) and select the plot just saved. The plots will be combined.

Table

Table produces a table of results according to the options selected in the **Performance** menu item in the **Parameters** menu for the design window.

The table has the usual cells with individual results but as it is produced the table has the attribute *read only* and so is protected from change. This is a safety feature to guard the integrity of the data.

There may be occasions when some editing of the data is necessary. The legend against **Design** right at the top of the table is a good place to put a very short note, for

example. For this reason the read only nature of the file can be changed. With the table window active select the Edit menu. There are two active items, **Copy Table** and **Read Only**. The read only status will be indicated by a tick to the left of the menu item. Select **Read Only** to toggle the status. When the tick is not visible, the table may be edited. It is good practice to return the status to read only after editing and immediately save the table.

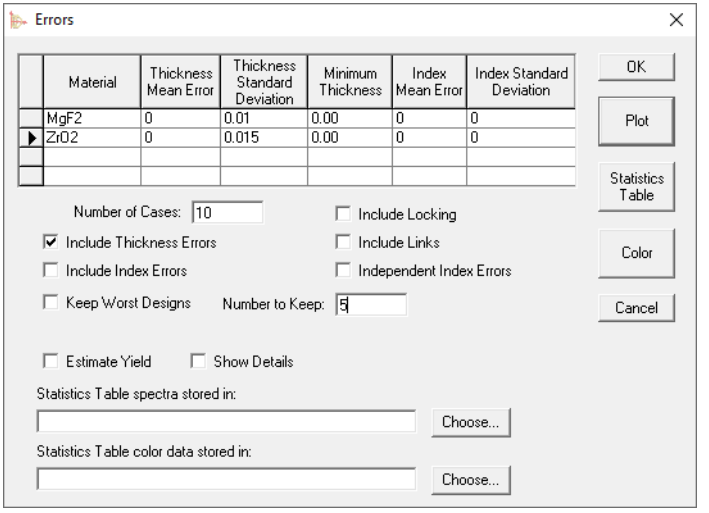
Copy allows the table to be copied to the clipboard and pasted subsequently into any other suitable application, especially a word processor.

More information about the table menus will be found in a later section.

Errors...

One of the most difficult areas in the design of optical coatings is the assessment of the sensitivity of the coating to errors. The errors in manufacture are generally rather larger than the first order approximations that can be readily handled by analytical techniques and so the most successful ones involve Monte Carlo modeling of the deposition process. Random errors drawn from suitable infinite populations are introduced and their effects over a large number of simulations are assessed. This is the technique on which the **Errors...** menu item is based.

Errors calculates successive performance curves for the design with thickness errors and refractive index errors drawn from a normal population. The parameters dialog box appears first.



Errors may be specified for both thickness and refractive index for each material in the design. For thickness errors, there are three parameters: **Thickness Mean Error**, **Thickness Standard Deviation** and **Minimum Thickness**. The **Thickness Mean Error** and **Thickness Standard Deviation** specify the statistical properties of the normal population from which the random numbers for thickness errors will be drawn. For layers that are thicker than the **Minimum Thickness**, the error will be applied as a proportion of the layer thickness. For example, to apply a thickness error where the standard deviation

is 2% of layer thickness and there are no systematic thickness errors, the following parameters are used:

Thickness Mean Error: 0
Thickness Standard Deviation: 0.02
Minimum Thickness: 0

In this case the thickness including error will be calculated as

ErrorThickness = LayerThickness + LayerThickness * RandomNumber

Another case is to apply an absolute error to the layer thickness that does not depend upon the thickness of the layer. For example, to apply a thickness error where the standard deviation is 2nm the following parameters can be used (providing no layer is thicker than 1000nm):

Thickness Mean Error: 0
Thickness Standard Deviation: 0.002
Minimum Thickness: 1000

In this case, the thickness including error will be calculated as:

ErrorThickness = LayerThickness + MinimumThickness * RandomNumber

With the values above, the standard deviation of the amount added to the layer thickness will be 1000 * 0.002 = 2 nm.

A combination of proportional and absolute errors can be achieved by correct setting of the minimum thickness. For example, to specify 2% thickness errors with a minimum thickness error standard deviation of 2nm, the following parameters would be used:

Thickness Mean Error: 0
Thickness Standard Deviation: 0.02
Minimum Thickness: 100

For layers thicker than 100nm, the thickness error will be calculated as

ErrorThickness = LayerThickness + LayerThickness * RandomNumber

For layers thinner than 100nm, the thickness error will be calculated as:

ErrorThickness = LayerThickness + MinimumThickness * RandomNumber

For layers thinner than 100nm, the standard deviation of the amount added to the layer thickness will be 100 * 0.02 = 2 nm

For refractive index errors, there are two parameters: **Index Mean** and **Index Standard Deviation**. The **Index Mean Error** and **Index Standard Deviation** specify the statistical properties of the normal population from which the random numbers for index errors will be drawn. For refractive index errors, the random number is added to the packing density of the layer to generate the perturbed refractive index for the layer, i.e.

ErrorPackingDensity = Packing Density + RandomNumber

Two checkboxes control the application of thickness and index errors. If **Include Thickness Errors** is checked, then thickness errors will be calculated. If **Include Index Errors** is checked, then refractive index errors will be calculated. Both types of error can included at the same time.

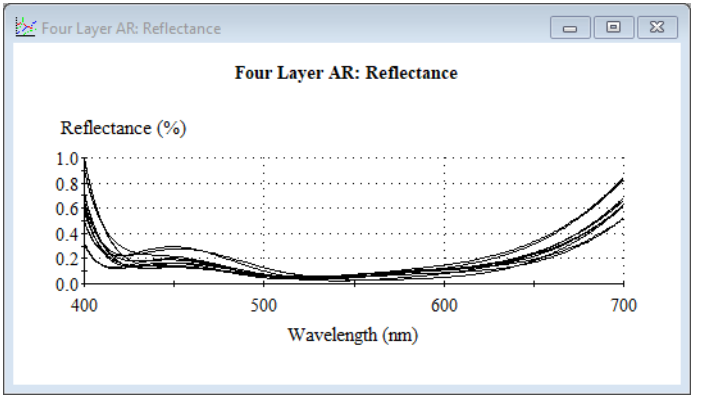
If **Include Locking** is checked, then only the layers that are not locked will have their thicknesses altered. If **Include Links** is checked, then the thickness of one of the layers in each set of linked layers will be randomly altered and then the other layers in the link set will have their thicknesses adjusted so that they have the same ratio of thicknesses to the randomly altered layer as in the original unperturbed design. For example, if layer 1 is 15nm thick and layer 2 is 30nm thick, and these layers are linked, then during Errors, layer 1 will be randomly altered and layer 2 will be set to be twice as thick as layer 1

If **Independent Index Errors** is not checked, then all layers of the material will have the same packing density error applied to them. If **Independent Index Errors** is checked, then different refractive index errors will be applied to each layer.

The **Number of Cases** is just the number of different curves with different random errors drawn from the specified populations.

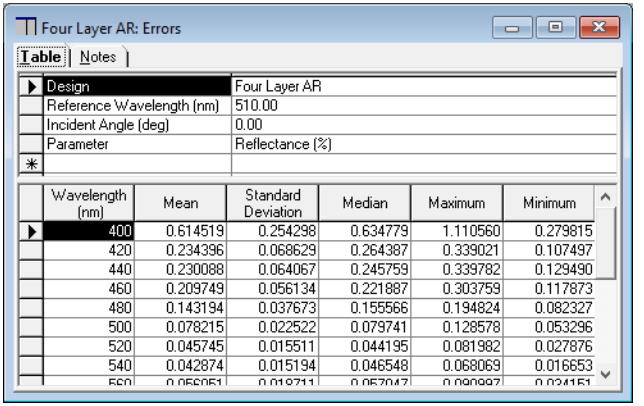
Sometimes it is useful to look at the worst designs generated where "worst" means has the largest merit figure. To keep the worst designs, check **Keep Worst Designs** and enter the maximum number of designs to be kept in **Number to Keep**. When the process is started a window will appear with a list of merit figures. These are the worst designs generated. Double-click on a merit figure to open the design that has that merit figure. When the list of merit figures window is closed, the worst designs that are not open or have not been saved will be discarded.

A numerical estimate of the yield given the random errors can be made by checking **Estimate Yield**. When the error calculations are performed a yield window will appear indicating the number of perturbed designs that meet the yield specification (the yield specification is created using the Yield Specification command in the Edit menu of a Design). For yield specifications with several tests, it will be difficult to determine where the designs did not meet the yield specification. Checking **Show Details** will change the output of Estimate Yield from showing the proportion of designs meeting the yield specification to a table showing, for each perturbed design the results of each yield specification. A yield specification that is not met by the design is highlighted in red. Double-clicking on an entry in the details table will open the corresponding perturbed design.



Once the correct parameters have been entered click the **Plot** button. The program will draw a series of curves each of which represents the performance of the coating with a different set of errors all drawn at random from the specified infinite populations with the parameters that have just been entered. By varying the error parameters and replotting an assessment of manufacturing tolerances can readily be made.

To see a table of statistics, click the **Statistics Table** button.



Wavelength (nm)	Mean	Standard Deviation	Median	Maximum	Minimum
400	0.614519	0.254298	0.634779	1.110560	0.279815
420	0.234396	0.068629	0.264387	0.339021	0.107497
440	0.230088	0.064067	0.245759	0.339782	0.129490
460	0.209749	0.056134	0.221887	0.303759	0.117873
480	0.143194	0.037673	0.155566	0.194824	0.082327
500	0.078215	0.022522	0.079741	0.128578	0.053296
520	0.045745	0.015511	0.044195	0.081982	0.027876
540	0.042874	0.015194	0.046548	0.068069	0.016653

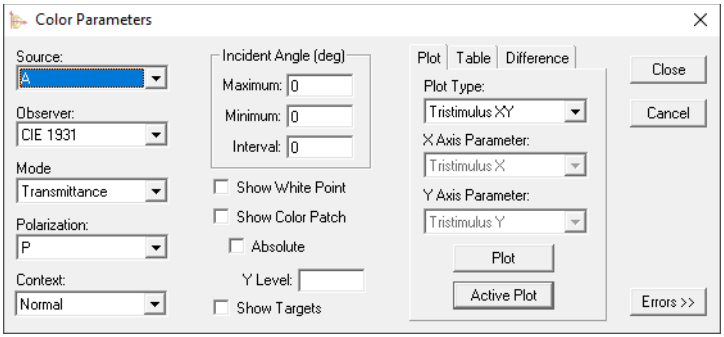
A new set of errors will be generated and the statistics of the resulting performance data will be calculated and displayed as shown in the table above. The statistics calculated are Mean, Standard Deviation, Median, Maximum and Minimum. If a filename is entered in the **Statistics Table spectra stored in** box, the calculated performance data will be stored in the file in CSV format. This data can then be manipulated by any program that reads csv files. The **Choose** button next to the box displays a file chooser for easier entry of the filename. If a filename is entered in the **Statistics Table color data stored in** box, the color parameters selected in the Table list of the color dialog (see below) will be stored in the file in CSV format. This data can then be manipulated by any program that reads csv files. The **Choose** button next to the box displays a file chooser for easier entry of the filename.

For convenience, the Errors dialog also has a **Color** button. Clicking this button will display the Color dialog (see below) with the error parameter part also displayed.

Color

The following color parameters are available: Tristimulus, Chromaticity, CIE L*a*b*, CIE L*u*v*, CIE L*u'v', Hunter LAB, CIE1960 u,v, Correlated Color Temperature (CCT), Reciprocal Correlated Color Temperature (RCCT), Dominant Wavelength (Wd), Complementary Wavelength (Wc), Excitation Purity (Pe) and Colorimetric Purity (Pc). For the CIE L*a*b* color space, the hue and chroma correlates are also calculated. For the CIE L*u*v* color space, the hue, chroma and saturation correlates are also calculated. Color difference in the CIE L*a*b* color space can be calculated, CIE76 and CIEDE2000 methods are available. The Coloring Rendering Index for a coating combined with a light source can also be calculated.

The dialog box that appears has several fields for completion.



Source lists the sources. The standard sources are CIE A, B, C, D55, D65, D75 and equal energy. Black body and other sources can readily be added especially if the Function Enhancement is present. Instructions are in the earlier section on Color.

Observer lists the sets of tristimulus values that are to be used. As supplied, these are CIE 1931 and CIE 1964. Again other observer definitions can be added if required.

Mode specifies whether the transmitted or reflected color will be calculated.

Polarization specifies the polarization to be used for oblique incidence calculations.

Context specifies the coating context to be used for the calculations.

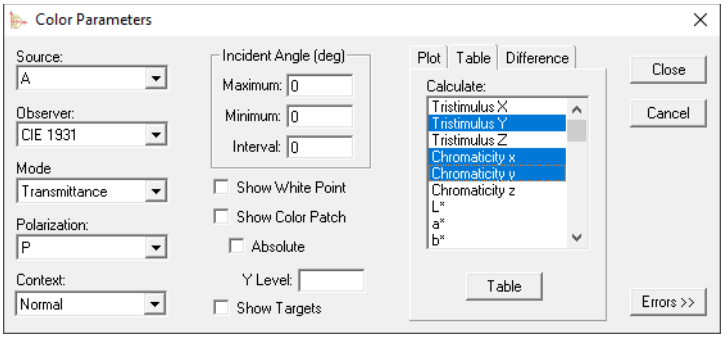
Incident Angle contains a set of three parameters that specify the range of incident angles and interval to be used in the calculation.

Show White Point places a symbol on the plot or creates a table entry that shows the coordinates of the source.

Show Color Patch creates a window that displays a visual impression of the color(s) of the coating.

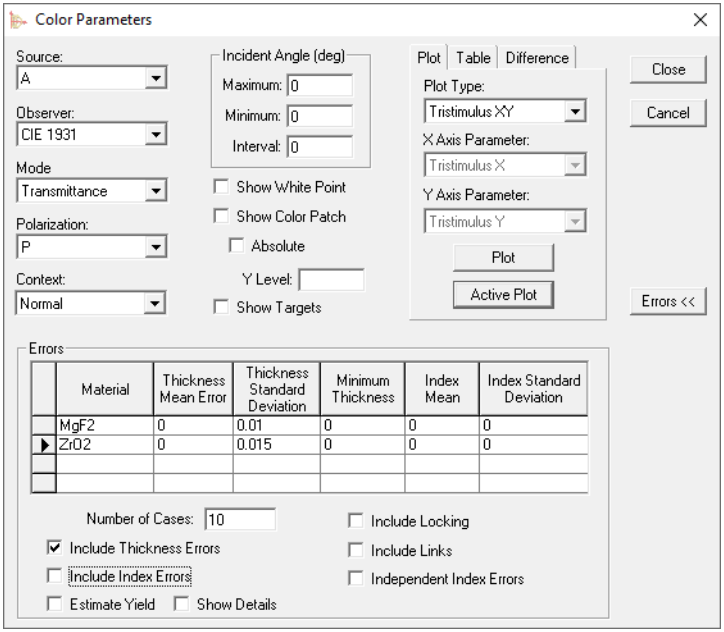
The **Plot** tab allows you to choose a standard plot or select two color parameters to plot. The standard plots available are: Tristimulus XY, Chromaticity xy, CIE 1976 UCS, CIE 1976 h*c*(ab), CIE 1976 h*c*(uv). The Chromaticity xy plot is plotted on a chromaticity diagram. The CIE 1976 UCS plot is plotted on a UCS diagram. The CIE 1976 h*c*(ab) and CIE 1976 h*c*(uv) plots are plotted on a polar diagram. If a Custom plot is selected, then the **X Axis Parameter** and **Y Axis Parameter** specify the color parameters to use in the plot. Clicking the **Plot** button causes the selected parameters to be plotted. Clicking the **Active Plot** button causes the parameters to be plotted in an Active Plot window. If **Show Color Patch** is checked, the color patch will also be active. See the Active Plot chapter (page 137) for more information on Active Plots.

The **Table** tab allows you to choose the color parameters to be included in the table output. Parameters are selected by clicking on them. Each selected parameter is highlighted in the list. In the figure below, the table will contain three parameters: Tristimulus X with Chromaticity x and y.



The **Difference** tab permits the calculation of color difference in the CIE L8a*b* color space. The reference color can be entered as either L*a*b* coordinates or the hue and chroma correlates L*c*h*. Clicking on Table will display the CIE76 and CIEDE2000 color differences.

Errors >> drops down an extra part of the form that allows you to see the effects of random thickness errors on the color of a coating in the same manner as the Errors command.



Please see the Errors command described earlier in this chapter for information on the error parameters.

If you do not wish to include the error variation in the color output, click the **Errors <<** button to close the error parameters part of the form. Plotting or generating a table with the errors part closed will calculate the color of the coating design without random variation.

Active Plot

This command starts an Active Plot using the current plot parameters. For more information on active plots, see the active plot chapter (page 137).

3D Plot

3D Plot initiates the plotting of performance in a 3D plot window. The aspects of performance and the range over which they are to be plotted have already been chosen under the item **3D Performance** in the **Parameters** menu.

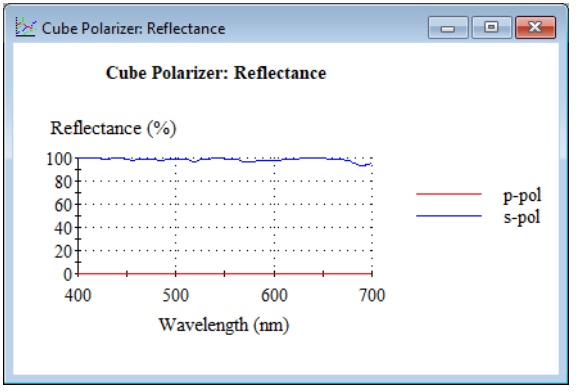
The 3D Plot window is now the active one and so the menu bar changes to reflect that. The principal changes are that the **Performance** and **Parameters** menus disappear and the choices under the others are limited.

Many aspects of the plot can be modified. The section on the 3D Plot Window later in this manual describes how 3D plots may be modified. Note that the performance data do not change when the 3D plot parameters are altered.

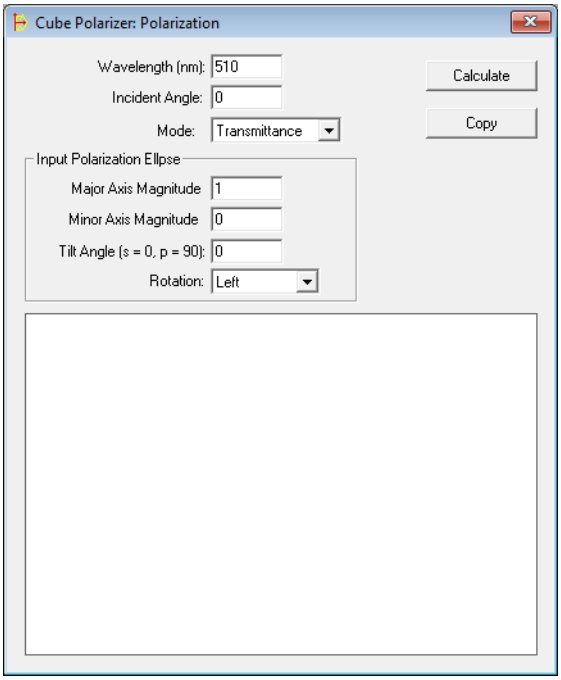
Polarization...

The Polarization tool allows you to visualize the effect of a coating on the polarization state of an incoming beam. The polarization state is specified as a ellipse with major and minor axis amplitudes together with a tilt angle that specifies the rotation of the ellipse major axis from the s-polarization plane For polarization states with a non-zero minor axis, the rotation of the polarization vector can be specified as either left-handed or right-handed. This rotation direction is specified looking in the direction of propagation of the beam.

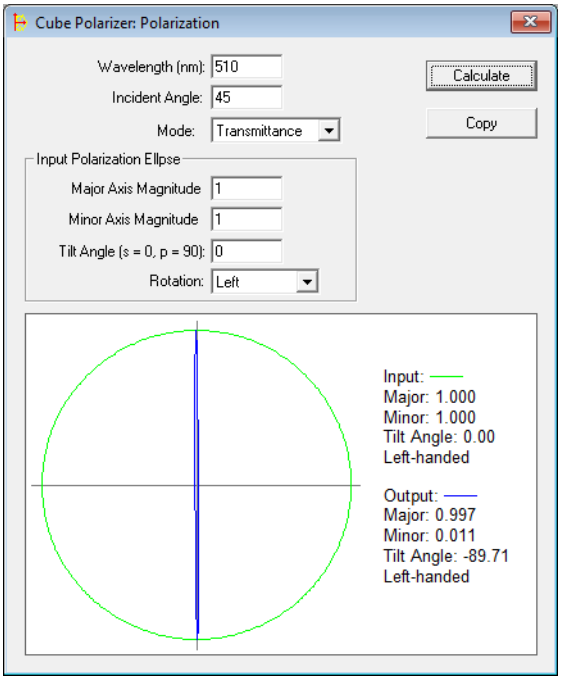
As an example, we will use the Cube polarizer design that is supplied with the software. The performance of the polarizer is:



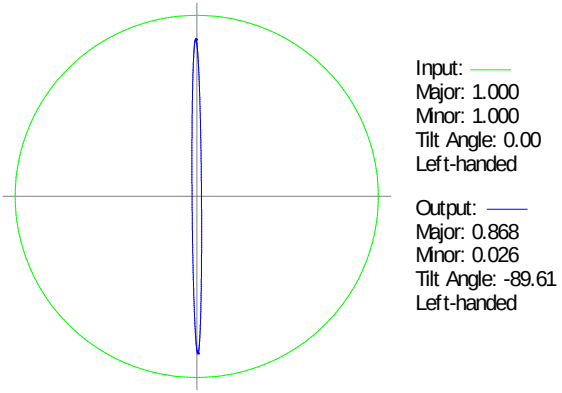
With the Design active, selecting **Polarization** from the **Performance** menu displays



For the input state, we will enter a left-circularly polarized beam, that is, equal major and minor axis magnitudes. Tilt angle does not apply to a circularly polarized beam so this parameter will be left at zero. We will consider transmittance at 45 degrees incident angle at a wavelength of 510nm. After entering the values and clicking **Calculate**, the following will be displayed.



As expected, transmission through the coating converts the circularly polarized beam into a relatively p-polarized beam. Clicking **Copy** copies the beam picture so that it may easily be inserted into a document:



Lock/Link Menu (Design)

Locking and Linking are constraints that are used in some of the refinement and synthesis procedures. A locked layer is excluded from any variation and remains constant

in both index and/or thickness. Layers that are linked together vary as a group in exactly the same manner. These constraints are useful both in the creation of a design where the structure is largely known but fine tuning has to be carried out on various parts and in reverse engineering for the investigation of possible process defects. There are also cases where coatings are to be designed to be deposited over already existing structures, the hard coating on spectacle lenses is an example.

Lock

Locking affects the way that the layers are treated in some of the refinement techniques. Layers may have their thickness locked, their packing density locked or both thickness and packing density locked. If a layer is thickness locked it retains its initial thickness throughout the operation. Similarly, if a layer is packing density locked, it retains its initial packing density throughout the refinement. To lock a group of layers they should first be selected by clicking in the selection box. **<Shift> click** will select a contiguous group of layers while **<Ctrl> click** will select a noncontiguous layer. Once the layers are selected, each successive use of the **Lock** command cycles the lock state of the layer through the three possible options: thickness locked (indicated by **d**), packing density locked (indicated by **n**) or thickness and packing density locked (indicated by **d, n**). Note that once the locking column appears in the design table, locking or unlocking of individual layers is probably more easily achieved simply by clicking on the locking cell to toggle the locking status. Thickness locking is very useful when it is known that the core of a coating should be unchanged. A good example is a quarterwave stack that is to be converted into an edge filter. Only the few outermost layers need be involved in any refinement.

Unlock

Unlock unlocks the selected layers. The remarks under **Lock** apply here also. It is easy to check that all layers are unlocked because then the lock column in the design table automatically disappears.

Link

Layers that are linked move together during refinement. There may be several different groups of layers in a particular design that are linked together. One linked group is distinguished from another by having a different reference number for the link. Layers with the number zero against them in the link column are unlinked. Those that are labeled 1 move together as a group. Those labeled 2 also move together but as a different group from those labeled 1, and so on. The number given to the link is that of the first layer that is involved in the linked group. Locked layers cannot form part of a link and a link must have more than one member. Sometimes a linked design may be edited so that the links move away from their original positions. Then a new and separate link may automatically be given the same designation as an existing link. In that case the new link numbers can be easily altered manually so that they can be distinguished from the earlier set.

Unlink

This cancels any links that apply to the selected group of layers. A good indication that all layers in a design are unlinked is that then the link column automatically disappears. If it does not then a residual link must exist somewhere in the design.

Lock All

This command changes the lock state of all layers. This is useful when just a few outermost layers are to be unlocked. Successive use of this command causes the lock state of all layers to cycle through the three possible options. All may be locked using this command and then the few that are to be refined may be manually unlocked.

Unlock All

This unlocks all layers in a design.

Link All Materials

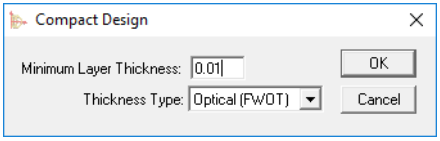
For each material used in a design, this command links all the layers in a design that use the same material. It is very useful in reverse engineering applications where, for example, you want to look at the effect of variations in tooling factor on the performance of a design.

Tools Menu (Design)

The Tools menu gives access to several devices for altering the coating design and also is a useful route to the editing of layer materials.

Compact Design

Compact Design will remove all layers of thickness less than a defined limit and close up the design. The layers are removed in a way that has minimum impact on the performance. The thinnest that meets the removal criterion is removed first and then the design is closed up. Then the design is resurveyed and the thinnest layer meeting the criterion removed, and so on.



Refine Design

The techniques available in the Essential Macleod are Simplex, (often called nonlinear simplex to distinguish it from a similarly named technique in linear programming), Optimac, Simulated Annealing, Conjugate Gradient, Quasi-Newton, Differential Evolution and Needle synthesis. Optimac can accomplish synthesis or refinement.

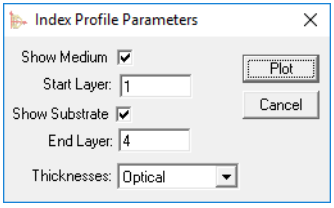
Simplex and Simulated Annealing also have the facility to refine in terms of layer thickness or of packing density, or of both. Packing density can be used in different ways either to simulate inhomogeneous layers or other production variations in reverse engineering, or simply to refine in terms of refractive index instead of thickness or even both simultaneously.

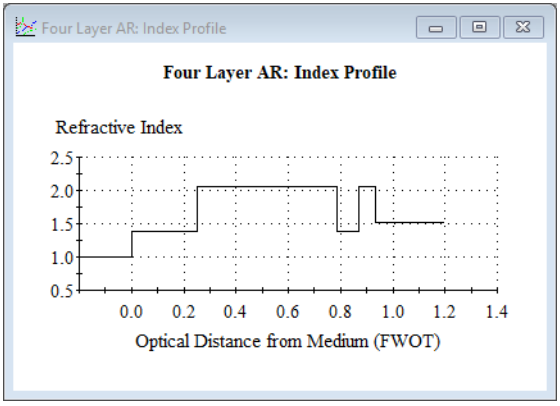
Selection of any of the techniques in this menu immediately initiates the refinement or synthesis process, unlike the corresponding command in the parameters menu that brings up first a parameters dialog box.

Refinement and synthesis are considered in greater detail below.

Index Profile...

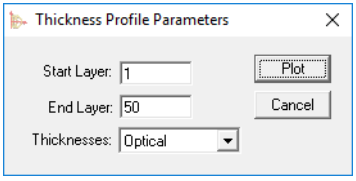
This produces a plot of refractive index against thickness in the chosen thickness units. **Start Layer** and **End Layer** are optional and, if the entire design is to be shown, a short length of substrate and incident medium are also optional. The following figure shows a quarter-half-quarter antireflection coating. In the index profile the incident medium is on the left and the emergent medium, or substrate, on the right

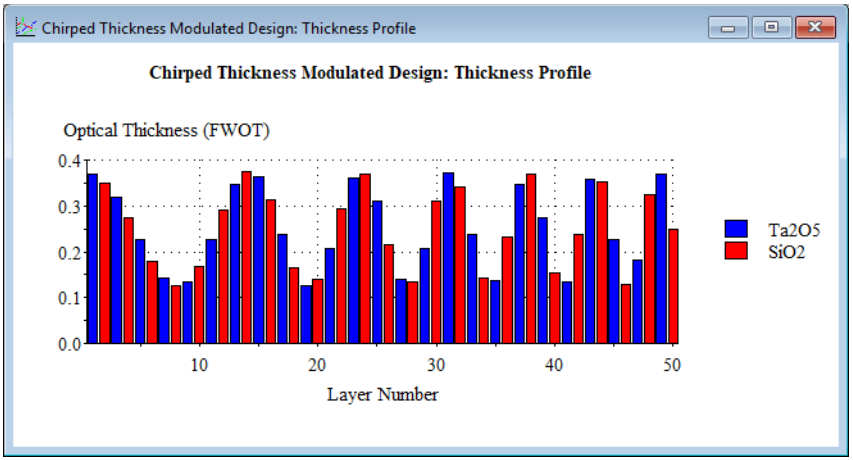




Thickness Profile...

This produces a plot of thickness against layer number in the chosen thickness units. **Start Layer** and **End Layer** specify the layer range to be plotted. The following plot shows a chirped thickness modulated coating where the modulation frequency increases with layer number.

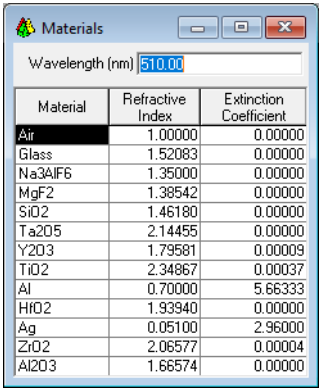




The modulation is readily apparent in the plot.

Materials

Selection of this item displays and activates the materials window for the current material database. The materials window and the operations that can be carried out on materials will be detailed below. Here we give just a brief account.



Materials may be chosen from this window for further examination, for editing, display and exporting.

Material names can be dragged in the window to change their order. For example the materials used most often may be arranged near the head of the list. Since this list determines the order in the small lists that are used for design editing it can be very useful in speeding up the design entry and editing process.

Options Menu (Design)

The **Options** Menu permits changes in certain aspects of the configuration of the package. These items are listed in greater detail above in the Applications Window Menu section.

General...

A dialog box permits the alteration of some of the details of the operation of the program. Note that although the materials folder is displayed, this is for reference only. The arrow to the right of the text box and the name of the materials folder within the box

are both grayed out. It is not permitted to change the current materials folder when a design is open. This dialog also permits you to change the display order of the layers.

Set as Default Design

The default design is the one that is created by the **New...** command under the **File** menu. Selecting this command copies the active design to the default design file for the current materials database. If the database is changed the default design will change with it. This means that the default design can always be appropriate to the particular database.

Window Menu (Design)

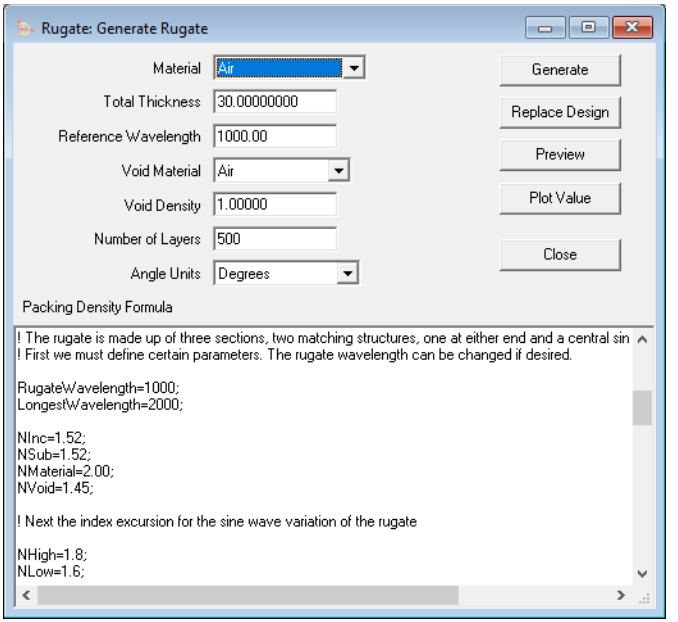
The **Window** menu has the same function throughout the package where it appears. It permits the organization of the presentation of the various open windows to be rearranged or to be switched from cascade to tile. The icons indicating reduced windows can be straightened up into rows. The various open windows are listed and can be brought to the front and activated by selecting the correct menu item.

Help Menu (Design)

This menu is identical throughout the package. It gives access to the on-line help facility and also displays a box with information about the program and about the installation. More information is given earlier under Essential Macleod Application Window.

Modeling a Rugate

In the Essential Macleod, a rugate coating is modeled as a set of layers where the packing density of each layer is varied through the set to provide the desired index profile. The **Generate Rugate** command in the Edit menu is a tool that simplifies the generation of the set of layers.



The limits of the index variation may easily be established by setting the **Material** parameter to a material that represents the highest refractive index that is present in the coating, setting the **Void Material** to a material that represents the lowest refractive index that is present in the coating and setting the **Void Density** to 1. As the packing density varies from 1 to 0, the refractive index will vary from the **Material** refractive index to the **Void Material** refractive index. Since the layer refractive indices are calculated using the packing density function, other relationships between packing density and refractive index can also be used (for example the valid packing density range may be 0 to 2 instead of 0 to 1).

The total thickness of the rugate structure is specified in optical by the **Total Thickness** value. The **Reference Wavelength** must also be specified. **Number of Layers** specifies the number of layers that are used to model the rugate structure. Increasing the number of layers improves the accuracy of the calculations at the expense of increased calculation time. A good starting point is to set the number of layers so that each layer is about one eighth of a wave thick at the shortest operating wavelength of the structure. To check the quality of the performance calculations, increase (or reduce) the number of layers and calculate the performance again. If there is little or no change in performance, then the number of layers is sufficient.

The Packing Density Formula is used to enter a set of statements that specify how the packing density varies through the set of layers. The formula consists of one or more statements. Each statement consists of an optional *Condition*, and an *Assignment*. A *Condition* is specified by an *Expression* followed by a colon (“:”) An *Assignment* is a *Variable* name followed by an equal sign (“=”) followed by an *Expression* and ends with a semi-colon (“;”). Any text after an exclamation point (“!”) is ignored up to the end of the line.

When a rugate structure is being generated, the statements in the Packing Density Formula are executed in order from top to bottom. If a statement has a *Condition*, then the *Assignment* is only executed if the value of the *Expression* in the *Condition* is not zero. If the statement does not have a *Condition*, then the *Assignment* is always executed. The *Assignment* calculates the value of the *Expression* and stores the value in the *Assignment Variable*. *Variables* are automatically created if they do not already exist. There are several special variables:

L	The current layer number. This variable cannot be modified. The first layer is numbered 1 and the last layer has the value **N**.
N	The number of layers as entered in the Number of Layers box. This variable cannot be modified.
TotalThickness	Total Thickness as entered in the Total Thickness box. This variable cannot be modified.
LayerThickness	The Thickness of one layer: (**TotalThickness** / **N**). This variable cannot be modified.
Thickness	Cumulative Thickness to center of current layer: (**L**-1) * **LayerThickness** + **LayerThickness** / 2. This variable cannot be modified.
ReferenceWavelength	Reference Wavelength as entered in the Reference Wavelength box. This variable cannot be modified.
PackingDensity	The Packing Density of the current layer. After all the statements have been executed, the current layer's packing density will be the value of this variable. This variable can be modified.

The following operators are supported in *Expressions*:

()	sub-expressions
^	power
*, /	multiplication, division
%	modulus (remainder)
\	integer divide
+, -	addition, subtraction
>, >=, <, <=, <>	logical comparison
&, |	logical "and", logical "or"

An operator that is listed on a line above another operator has a higher precedence. The following functions are also supported (they are not case sensitive): Abs, Sin, Cos, Tan, ACos, ASin, Atn, Log, Log10, Exp, Sqr, Int, Frac, Ceil, and Floor. Trigonometric functions accept and return angles expressed in radians or degrees, depending on the setting of **Angle Units**.

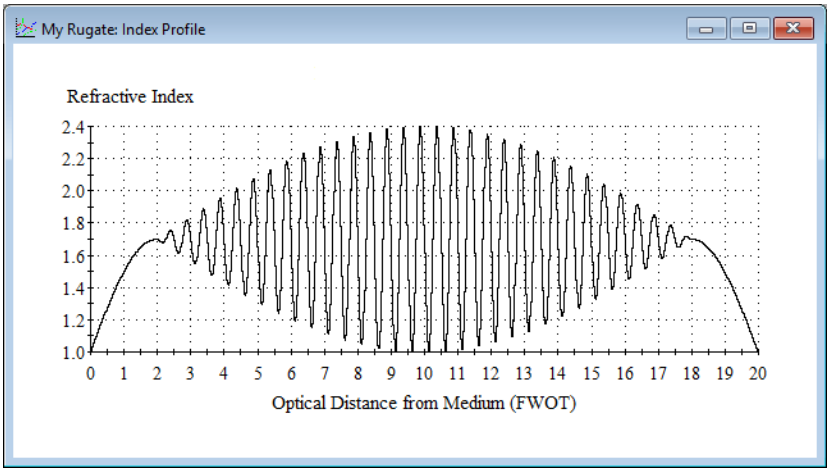
For example, the formula:

PackingDensity = (1 + sin(360 * L/N))/2;

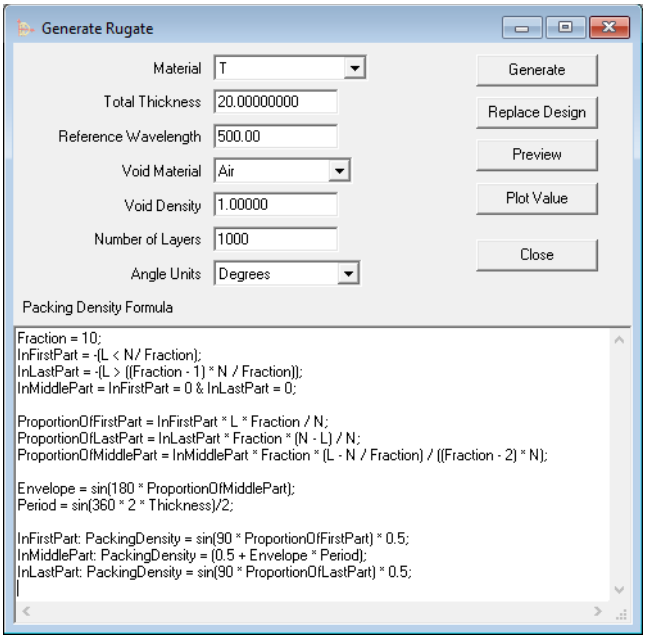
generates a rugate structure consisting of a single period of a sine wave.

Click **Preview** to generate an index profile plot of the rugate structure. This allows you to verify that the correct structure has been generated. The rugate structure can be made available to the design in two ways: Clicking **Generate** will put the layers of the rugate structure onto the clipboard. These layers can be pasted into any design in the normal way. Clicking **Replace Design** will cause the current design's layers to be completely replaced with the layers of the rugate structure. Selecting a variable name in the Packing Density Formula and then clicking **Plot Value** will display a plot showing the value of the variable as a function of thickness. This is useful for making sure that the variable's value is set correctly during rugate generation.

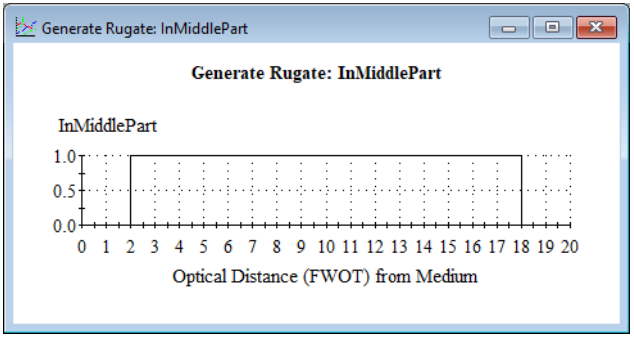
Here is a more complicated example. In this example, we want to generate the following refractive index profile:



There are three parts to this rugate. The first part is the rise in refractive index from 1.0 to 1.7. This is achieved by the first 90 degrees of a sine wave profile. The second part is a sine wave profile of 32 cycles modulated by a half sine wave profile. The last part is a fall in refractive index from 1.7 to 1. This is achieved by the following Generate Rugate form:



The first four lines set up the three parts of the rugate. The first and last parts are each one tenth of the total thickness and the second part is eight tenths of the total thickness. **InFirstPart** is 1 during the first tenth and 0 elsewhere. **InLastPart** is 1 during the last tenth and 0 elsewhere. **InMiddlePart** is 1 when both **InFirstPart** and **InLastPart** are 0 and 1 elsewhere. Selecting **InMiddlePart** and then clicking **Plot Value** gives the following plot:



ProportionOfFirstPart, **ProportionOfMiddlePart** and **ProportionOfLastPart** start at 0 and linearly increase to 1 in each appropriate part.

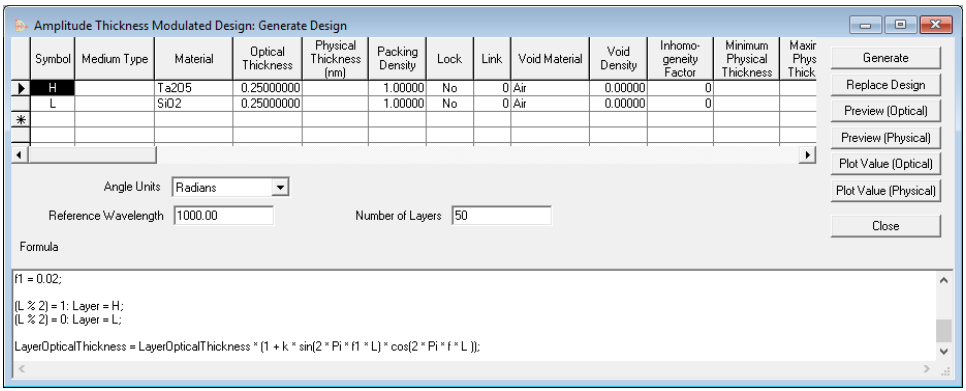
The envelope for the middle part is generated by a sine function that uses **ProportionOfMiddlePart** to generate an angle that varies from 0 to 180 degrees.

The periodic component is generated by another sine function whose period is one half an optical thickness. The periodic component is scaled so that it varies from –0.5 to +0.5 – a total range of 1.

The last three statements generate the packing density variation. These statements use the *Condition* component to control which statement provides the packing density as a function of thickness. For the first part, the first 90 degrees of the sine function are used to raise the packing density from 0 to 0.5 (the midpoint of the packing density range used here). In the middle part, the periodic component is multiplied by the envelope and the result is then shifted up by 0.5 to give a packing density that varies from 0 to 1. The last part is generated by a sine function starting at 90 degrees and reducing to 0.

Generating Complex Designs

In the Essential Macleod, the Formula tool is used to generate designs with regular features. Some designs have more complex features that cannot be expressed by using Formula, such as chirped reflectors. For these designs, the Generate Design tool can be used to generate the layers in the design.



A Generate Design definition consists of default layer parameters represented by single letter symbols, the number of layers in the design and a Formula that specifies the parameters of each layer as a function of layer number.

The Formula is used to enter a set of statements that specify how the layer parameters vary through the set of layers. The formula consists of one or more statements. Each statement consists of an optional *Condition*, and an *Assignment*. A *Condition* is specified by an *Expression* followed by a colon (":") An *Assignment* is a *Variable* name followed by an equal sign ("=") followed by an *Expression* and ends with a semi-colon (";"). Any text after an exclamation point ("!") is ignored up to the end of the line.

When a design is being generated, the statements in the Formula are executed in order from top to bottom. If a statement has a *Condition*, then the *Assignment* is only executed if the value of the *Expression* in the *Condition* is not zero. If the statement does not have a *Condition*, then the *Assignment* is always executed. The *Assignment* calculates the value of the *Expression* and stores the value in the *Assignment Variable*. *Variables* are automatically created if they do not already exist. There are several special variables:

L	The current layer number. This variable cannot be modified. The first layer is numbered 1 and the last layer has the value **N**.
N	The number of layers as entered in the Number of Layers box. This variable cannot be modified.
OpticalThickness	The total optical thickness of the design excluding the current layer. This variable cannot be modified.
PhysicalThickness	The total optical thickness of the design excluding the current layer. This variable cannot be modified.
LayerOpticalThickness	The optical thickness of the current layer.
LayerPhysicalThickness	The physical thickness of the current layer.
LayerLocked	The lock state of the current layer. A value of 0 means the layer is not locked. A value of –1 means the layer is locked.
LayerLink	The link number of the current layer.
LayerPackingDensity	The Packing Density of the current layer.
LayerVoidDensity	The Void Density of the current layer.
LayerN	The refractive index of the current layer. This variable cannot be modified.
LayerK	The extinction coefficient of the current layer. This variable cannot be modified.
MaterialN	The refractive index of the current layer material. This variable cannot be modified.
MaterialK	The extinction coefficient of the current layer material. This variable cannot be modified.
VoidMaterialN	The refractive index of the current layer void material. This variable cannot be modified.
VoidMaterialK	The extinction coefficient of the current layer void material. This variable cannot be modified.
Layer	This is used to initialize the parameters of the layer. It should be used before any layer parameters are modified.
Thickness	Cumulative Thickness to center of current layer: (**L**-1) * **LayerThickness** + **LayerThickness** / 2. This variable cannot be modified.
ReferenceWavelength	Reference Wavelength as entered in the Reference Wavelength box. This variable cannot be modified.

PackingDensity	The Packing Density of the current layer. After all the statements have been executed, the current layer's packing density will be the value of this variable. This variable can be modified.
InhomogeneityFactor	The Inhomogeneity Factor of the current layer. After all the statements have been executed, the current inhomogeneity factor will be the value of this variable. This variable can be modified.
MinimumPhysicalThickness	The Minimum Physical Thickness for the current layer. After all the statements have been executed, the current layer's minimum physical thickness will be the value of this variable. This variable can be modified.
MaximumPhysicalThickness	The Maximum Physical Thickness for the current layer. After all the statements have been executed, the current layer's maximum physical thickness will be the value of this variable. This variable can be modified.
MinimumOpticalThickness	The Minimum Optical Thickness for the current layer. After all the statements have been executed, the current layer's minimum optical thickness will be the value of this variable. This variable can be modified.
MaximumOpticalThickness	The Maximum Optical Thickness for the current layer. After all the statements have been executed, the current layer's maximum optical thickness will be the value of this variable. This variable can be modified.

The following operators are supported in *Expressions*:

()	sub-expressions
^	power
*, /	multiplication, division
%	modulus (remainder)
\	integer divide
+, -	addition, subtraction
>, >=, <, <=, <>	logical comparison
&, |	logical "and", logical "or"

An operator that is listed on a line above another operator has a higher precedence. The following functions are also supported (they are not case sensitive): Abs, Sin, Cos, Tan, ACos, ASin, Atn, Log, Log10, Exp, Sqr, Int, Frac, Ceil, and Floor. Trigonometric functions accept and return angles expressed in radians or degrees, depending on the setting of **Angle Units**.

For each layer generated, the formula must perform a layer initialization as follows:

Layer = <symbol>

Where symbol is a defined symbol in the table shown at the top of the form.

For example, the formula:

```
Odd = ((L % 2) =1);
Even = ((L % 2) = 0);
Odd: Layer = L;
Even: Layer = H;
```

will generate an design of alternating H and L layers with no modifications to the layer parameters.

Click **Preview (Optical)** to generate an index profile plot of the design as a function of optical thickness. Click **Preview (Physical)** to generate an index profile plot of the design as a function of physical thickness. These commands allow you to verify that the correct structure has been generated. The design can be made available in two ways: Clicking **Generate** will put the layers of the design onto the clipboard. These layers can be pasted into any design in the normal way. Clicking **Replace Design** will cause the current design's layers to be completely replaced with the layers of the formula. Selecting a variable name in the Formula and then clicking **Plot Value (Optical)** or **Plot Value (Physical)** will display a plot showing the value of the variable as a function of optical thickness or physical thickness respectively. This is useful for making sure that the variable's value is set correctly during design generation.

This example shows the implementation of an amplitude thickness modulated design presented in Chapter 3 of "Thin Film Design Modulated Thickness and Other Stopband Design Methods by Bruce E. Perilloux ISBN: 0-8194-4525-8 Pub SPIE Press 2002. The function for modulating the thickness is given as:

$$T(L) = T_{AVG}[1 + k' \sin(2\pi f_1 L) \cos(2\pi f L)]$$

In the Generate Design tool, this function appears as:

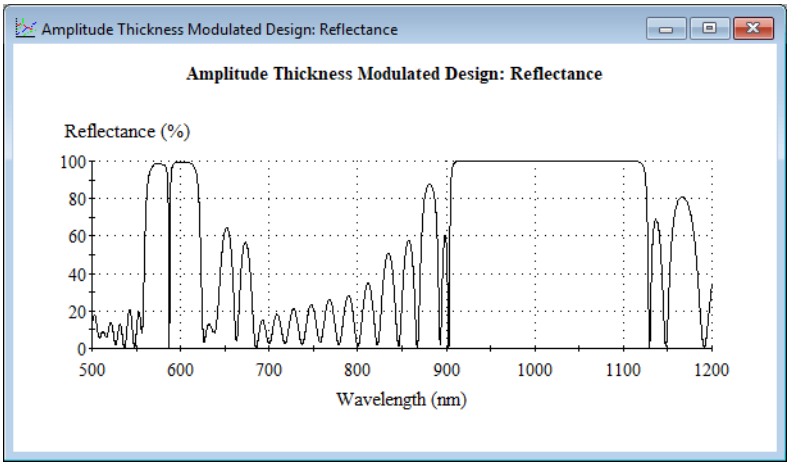
```
Pi = 3.1415926;
k = 0.5;
f = 0.358;
f1 = 0.02;

(L % 2) = 1: Layer = H;
(L % 2) = 0: Layer = L;

LayerOpticalThickness = LayerOpticalThickness * (1 + k* sin(2 * Pi * f1 * L) * cos(2 * Pi * f* L ));
```

The first four lines define constants for the formula. The next two lines specify that the design is made from alternating layers of H and L material. H material is used on the odd numbered layers and L material is used on the even numbered layers. The final line performs the modulation function. The optical thickness of the layer is modified by the modulation function.

A 50 layer design using Ta2O5 for the H material and SiO2 for the L Material, with the optical thickness in the table set at 0.25 at a reference wavelength of 1000nm produces the following reflectance performance:



Contexts

Contexts are used to specify the behavior of Agile Materials. An Agile Material is a material whose optical constants depend upon the Context. An Agile Material has a name and for each Context, a material name. When a calculation is performed using a particular Context, the optical constants of the agile material are those of the corresponding material in the Context.

Contexts are used during performance calculation and during refinement. Using Contexts, it possible to refine designs for production on multiple substrates, refine designs for production using a range of different real materials. This includes producing a single design for manufacture in coating plants that produce different optical constants for the same raw material.

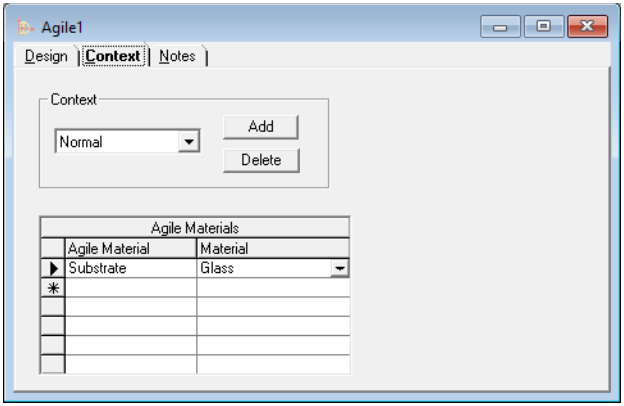
Agile1

Design | Context | Notes

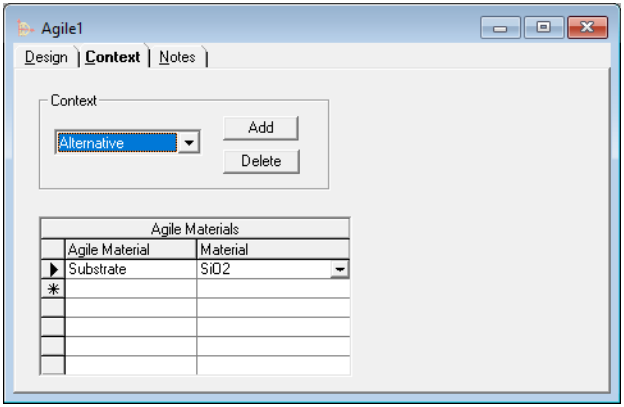
Incident Angle (deg)	0.00
Reference Wavelength (nm)	510.00

	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
	Medium	Air	1.00000	0.00000		
	1	SiO2	1.46180	0.00000	0.25160196	87.78
	2	Ta2O5	2.14455	0.00000	0.29153216	69.33
	3	SiO2	1.46180	0.00000	0.01742698	6.08
	4	Ta2O5	2.14455	0.00000	0.18468329	43.92
	5	SiO2	1.46180	0.00000	0.12562900	43.83
	6	Ta2O5	2.14455	0.00000	0.04242838	10.09
	7	SiO2	1.46180	0.00000	0.29921085	104.39
▶	Substrate	Substrate: Glass	1.52083	0.00000		
					1.21251262	365.42

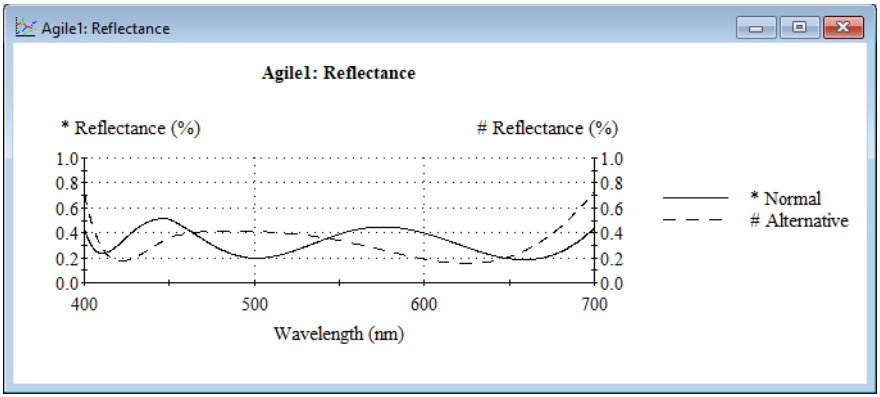
The design above is an antireflection coating that has been optimized for Glass and Silica substrates. This Design has one agile material: Substrate. To see the specifications for Substrate, click on the **Context** tab.



The Context that is shown is the Normal context. In this Context, the Agile Material Substrate has the optical constants of the material Glass. You can use the dropdown arrow to select a different Context.



In the Context named Alternative, the Agile Material Substrate has the optical constants of the Material SiO2. By specifying different contexts, the properties of the coating on Glass and on SiO2 can be calculated. The performance parameters dialog (**Parameters** menu -> **Performance**) allows you to specify a Context when calculating performance, so, for example, you can display the performance of the coating on both substrates on a single plot.



A Context can also be specified for each target in a refinement specification. To show the Context, select **Display Setup** from the **File** menu when the Targets window is active. Select the **Context** item and then click **Close**. You can now set the Context for each target.

A Design always has one Context. When a design is created, this Context is named Normal. You can add Contexts to a design by clicking the **Add** button in the Context tab. Enter the name of the new Context in the dialog that appears and click **OK**. Agile Materials are entered by typing the desired name in the Agile Material column. The optical constants to be used for the displayed Context are selected by choosing from the drop list in the Material column. There is no restriction to the number of Agile Materials that may be defined in a design.

In the Design editor, the Agile Materials are displayed at the top of the materials list. The displayed optical constants are those of the first Context. Contexts are only used in the Design editor. In the rest of the Essential Macleod where a design file is used, the first Context is used to specify the optical constants of the Agile Materials., the other Contexts are not used.

Inhomogeneity Factor

Inhomogeneity is a variation of optical properties across the film, most commonly in terms of the refractive index. There is no general analytical solution to the calculation of the effects of inhomogeneity. Accurate calculation involves the representation of the variation as a series of thin discrete layers of appropriately varying properties. Two tools that assist in preparing for such precise calculations are Graded Layers and Generate Rugate… However, implicit in the use of these tools is the existence of many additional layers, hidden in the case of Graded Layers, that add time to the calculations. There are many occasions when the inhomogeneity represents only a quite small correction to the properties of a discrete layer and a calculation technique with no reduction in speed is appropriate. This is the purpose of the inhomogeneity factor. The use of this factor involves a small modification to the basic characteristic matrix for the thin film rather than its replacement by a series of layers. This permits rapid calculation in Reverse Engineer and in the refinement and synthesis tools.

The change in refractive index across the layer is given by Inhomogeneity Factor * Layer Refractive Index. The refractive index at the medium end of the layer is given by Layer Refractive Index * (1 - Inhomogeneity Factor/2). The refractive index at the substrate end of the layer is given by Layer Refractive Index * (1 + Inhomogeneity Factor/2). A positive inhomogeneity factor indicates that the refractive index is increasing in the direction of the substrate. A negative inhomogeneity factor indicates that the refractive index is falling in the direction of the substrate.

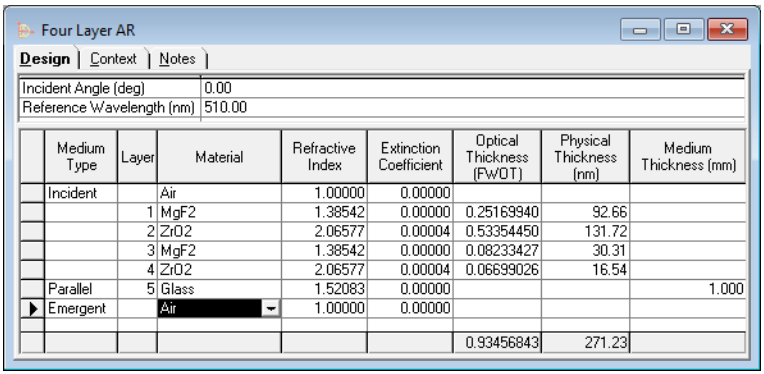
The model used to calculate the effects of the inhomogeneity is based on that given by: Abelès F., 1950 "Recherches sur la propagation des ondes electromagnetiques sinusoïdales dans les milieus stratifies. Application aux couches minces." *Ann Phys*. **5** pp596-640. It must be emphasized that this model involves some important limitations. The effect of the inhomogeneity must be small compared with the other interference properties of the layer and the variation of index through the layer should be slow and uniform to avoid any additional influence of the actual profile. Then the Abelès model cannot handle inhomogeneities in layers less than a quarterwave in optical thickness and so our model must accommodate a switch when a layer becomes less than that. A discontinuity that appears at around a quarterwave thickness of the appropriate layer is a sign that the model is being used outside its range of validity and that one of the alternative and precise techniques already mentioned must be used instead. In most cases an inhomogeneity factor in the range ±0.2 will be found to work well. Care should be exercised with larger factors.

Thick Layers

In a design, thin layers support coherent beam combination. Thick layers support incoherent beam combination, that is, there is no interference between the beams in a thick layer. A thick layer in a Design is identical to a medium in a Stack (see the Stack chapter for more information). In a Stack, it is possible to specify a Substrate – this defines the internal transmittance of the medium. The name of the substrate need not be the same as the name of the medium material. When a thick layer is used in a design, the name of the Substrate must be the same as the name of the Material. During calculations, if a Substrate of the same name as the Material cannot be found, a warning message is displayed and the thick layer will be assumed to be lossless, that is, it has an internal transmittance of 100%. A thick layer may be either **Parallel** or **Wedged**. A **Parallel** thick layer includes the complete infinite series of backward and forward propagating beams. A **Wedged** thick layer only includes the beam that passes straight through and the beams that are reflected just once at each surface. When a design contains one or more thick layers the calculations available are restricted to those available for a Stack and the Analysis functions are no longer available.

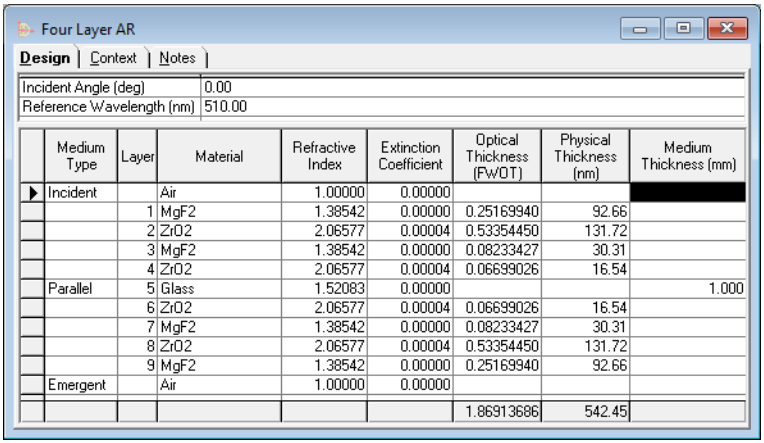
To create a thick layer in a Design, the Medium Type and Medium Thickness columns must be visible. To display these columns, use **File** -> **Display Setup** -> to make them visible. If the Medium Type is blank, this means that the layer is a normal thin layer. When Medium Type shows Parallel or Wedged, then the layer is treated as a thick layer with the appropriate beam combination. The thick layer thickness is entered in the Medium Thickness column. Note that a thick layer of zero thickness breaks the beam coherency between any surrounding thin layers, that is, it can be regarded as being lossless with a thickness whose actual value is unimportant.

As an example the design below shows the Four Layer AR design on a Glass substrate with Air as the emergent medium.



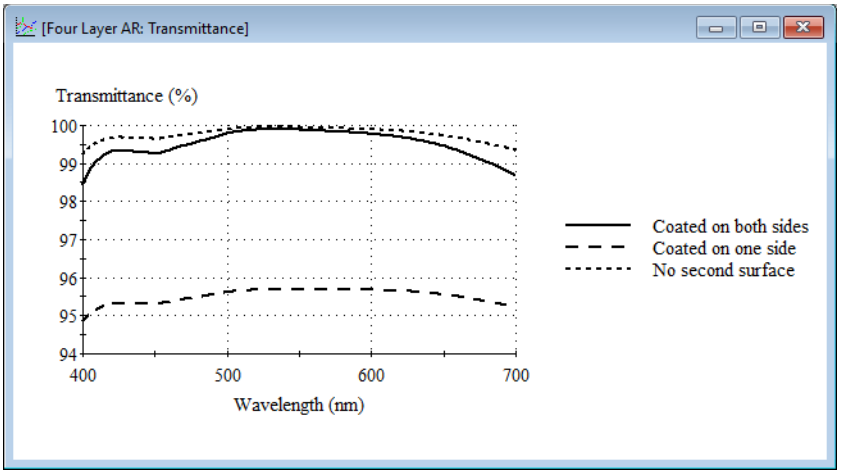
	Medium Type	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)	Medium Thickness (mm)
	Incident		Air	1.00000	0.00000			
		1	MgF2	1.38542	0.00000	0.25169940	92.66	
		2	ZrO2	2.06577	0.00004	0.53354450	131.72	
		3	MgF2	1.38542	0.00000	0.08233427	30.31	
		4	ZrO2	2.06577	0.00004	0.06699026	16.54	
	Parallel	5	Glass	1.52083	0.00000			1.000
▶	Emergent		Air	1.00000	0.00000			
						0.93456843	271.23	

This models a slab of glass 1mm thick with the AR coating applied to one side. To model the coating applied to both sides of the thick layer, the thin layers can be copied and pasted to the other side of the thick layer. To correctly orient the pasted layers they will need to be selected and reversed using the **Reverse Layers** command in the **Edit** menu.

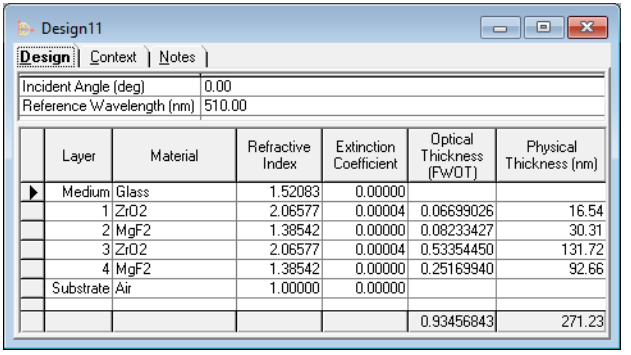


	Medium Type	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)	Medium Thickness (mm)
▶	Incident		Air	1.00000	0.00000			
		1	MgF2	1.38542	0.00000	0.25169940	92.66	
		2	ZrO2	2.06577	0.00004	0.53354450	131.72	
		3	MgF2	1.38542	0.00000	0.08233427	30.31	
		4	ZrO2	2.06577	0.00004	0.06699026	16.54	
	Parallel	5	Glass	1.52083	0.00000			1.000
		6	ZrO2	2.06577	0.00004	0.06699026	16.54	
		7	MgF2	1.38542	0.00000	0.08233427	30.31	
		8	ZrO2	2.06577	0.00004	0.53354450	131.72	
		9	MgF2	1.38542	0.00000	0.25169940	92.66	
	Emergent		Air	1.00000	0.00000			
						1.86913686	542.45	

The plot below shows the transmittance of the three designs. The “No second surface” curve shows the performance of the design only with no thick layer, that is, it shows the transmittance into the substrate. The “Coated on one side” curve shows the transmittance of the glass substrate with the coating applied to one surface. This is the transmittance you would expect to measure. The “Coated on both sides” curve shows the glass substrate with the coating applied to both surfaces.



To extract a contiguous set of thin layers from a design containing thick layers, select a layer in the contiguous set and then select the **Create Design** command in the **Edit** menu. This will create a new design containing the contiguous layers. The Medium and Substrate are set to the surrounding thick layers in the original design. The design below shows the result of **Create Design** when layer 8 of the double-sided design above was selected. Note that the orientation of the layers is the same as in the source design. To change the orientation of the design, use the **Reverse Design** command in the **Edit** menu. With the thick layers removed, the Analysis commands and phase calculations can now be performed.



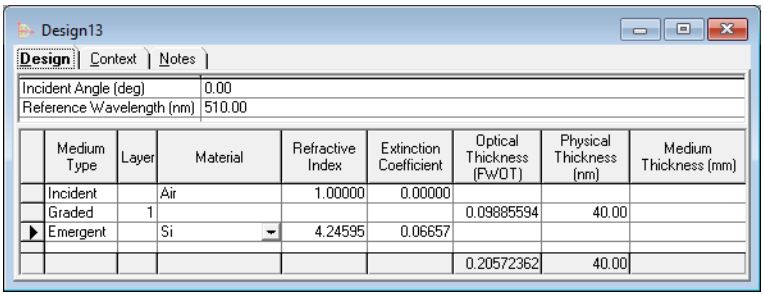
	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
▶	Medium	Glass	1.52083	0.00000		
	1	ZrO2	2.06577	0.00004	0.06699026	16.54
	2	MgF2	1.38542	0.00000	0.08233427	30.31
	3	ZrO2	2.06577	0.00004	0.53354450	131.72
	4	MgF2	1.38542	0.00000	0.25169940	92.66
	Substrate	Air	1.00000	0.00000		
					0.93456843	271.23

Graded Layers

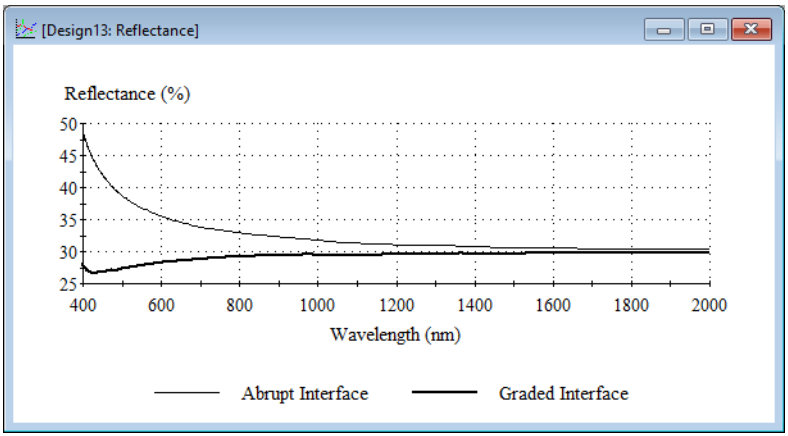
A graded layer provides a smooth transition in refractive index (and optionally extinction coefficient) from one layer to the next. This smooth transition can be used to model inter-layer diffusion and rough surfaces provided that the scale of the roughness is much smaller than the shortest wavelength of interest. The only parameter that can be specified for a graded layer is its thickness. The thickness may be specified as a physical thickness, an optical thickness or a geometric thickness. The layers surrounding the

graded layer define the optical constants at each end of the graded layer. The optical constants vary linearly with physical thickness from one end of the graded layer to the other.

A layer is specified as graded in the **Medium Type** column. If this column is not visible in the Design window, use **File** -> **Display Setup** -> **Medium** to make it visible. To make a layer graded, select **Graded** in the **Medium Type** cell. For example, the Design window below shows a silicon substrate with a 40nm thick graded interface to air.



The plot below compares the reflectance of the graded interface to the simple abrupt interface.



Scatter Layers

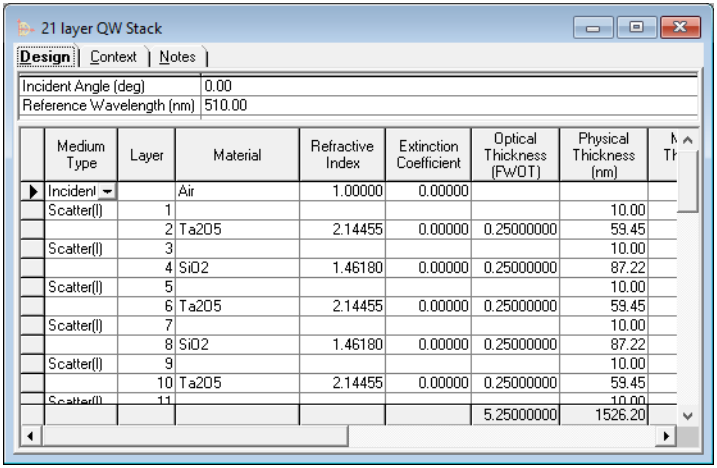
A scatter layer models the effect of rough layers on the specular performance of a design. There are two type of scatter layers available: a short range scatter layer denoted Scatter(s) and a long range scatter layer denoted Scatter(l).

The short range scatter layer models scattering that would be seen where the roughness of the layer is very small compared to the wavelengths of interest. This is achieved by using a graded layer. The difference between the Scatter(s) layer and the

graded layer described above is that during calculations, the thickness of the Scatter(s) layer is removed from the preceding layer (in the direction of the substrate). Thus you do not have to alter the non-scattering part of the design when adding the scatter layers. Accordingly, the thickness of the scatter layers does not appear in the total thickness for the design.

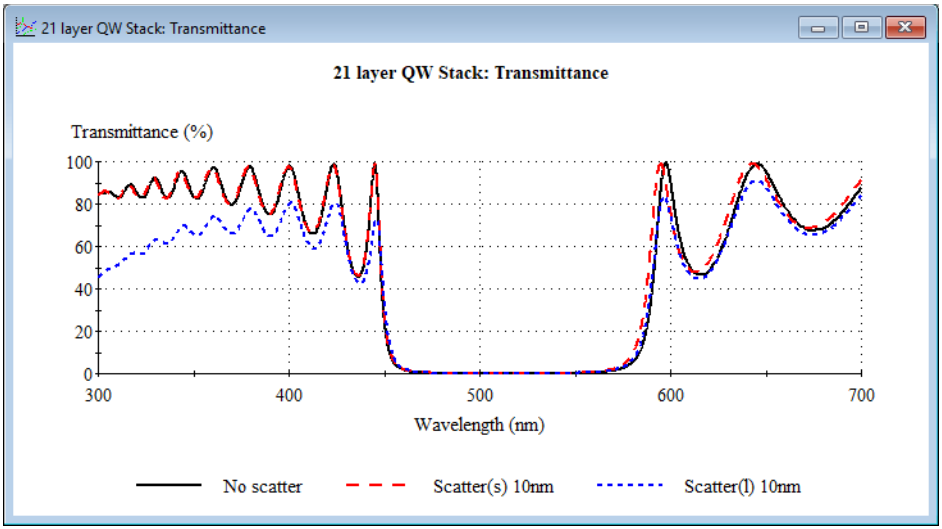
The long range scatter layer models scattering according to “Single-layer model for surface roughness” by C. K. Carniglia and D.G. Jensen in Applied Optics Volume 41 Number 16 June 2002. In this model, the scatter layer uses an intermediate material with extinction coefficient to reduce both transmittance and reflectance. Again the thickness of the scatter layer is removed from the thickness of the preceding layer during calculations.

A layer is specified as a scatter layer in the **Medium Type** column. If this column is not visible in the Design window, use **File** -> **Display Setup** -> **Medium** to make it visible. To make a layer a scatter layer, select **Scatter(s)** in the **Medium Type** cell for a short range scatter layer and **Scatter(l)** for a long range scatter layer. For example, the Design window below shows a quarterwave stack with scatter layers at each layer interface. The thickness of each scatter layer should be set to twice the rms roughness. The Edit menu for the Design window contains commands for quickly adding and removing scatter layers from a design.



	Medium Type	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)	M Th
▶	Incident		Air	1.00000	0.00000			
	Scatter(l)	1					10.00	
		2	Ta2O5	2.14455	0.00000	0.25000000	59.45	
	Scatter(l)	3					10.00	
		4	SiO2	1.46180	0.00000	0.25000000	87.22	
	Scatter(l)	5					10.00	
		6	Ta2O5	2.14455	0.00000	0.25000000	59.45	
	Scatter(l)	7					10.00	
		8	SiO2	1.46180	0.00000	0.25000000	87.22	
	Scatter(l)	9					10.00	
		10	Ta2O5	2.14455	0.00000	0.25000000	59.45	
	Scatter(l)	11					10.00	
						5.25000000	1526.20	

The plot below compares the reflectance of the quarterwave stack with short range scatter and long range scatter using an rms roughness of 5 nm (that is a layer thickness of 10 nm) for each layer


21 layer QW Stack: Transmittance
21 layer QW Stack: Transmittance
Transmittance (%)
100
80
60
40
20
0
300
400
500
600
700
Wavelength (nm)
No scatter
Scatter(s) 10nm
Scatter(l) 10nm

PLOT WINDOW

The Plot window is where the plots are produced. Several of these may be open at any one time. They may also be reduced to icons by using the minimize button.

The package uses adaptive plotting so that it tries to include all the fringes, even very tight ones, in a plot.

When the plot window is active you can hold down the **<Alt>** key and use the left mouse button to display markers on the plot and have x -and y- coordinates of the markers displayed on the plot. If you wish to remove the markers, click **Clear Cursor** in the Edit menu, or right –click on the mouse when it is over the plot and select **Clear Cursor** from the menu that appears.

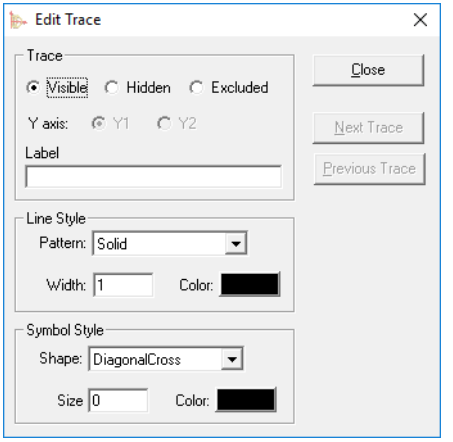
A plot can be dragged from one plot window to another. Dragging a plot and dropping it onto another plot window adds the dragged plot to the plot contained in the destination window. Columns of tables can also be dragged onto a plot. See the table window chapter for more details.

Plot Zoom

To zoom in to a particular area of a plot, hold the **<Shift>** down and whilst holding down the left mouse button, drag the mouse to define the zoom area. When you release the left mouse button, the plot will be redrawn so that the zoom area fills the plot. To reset the plot so that it shows all the data, press the letter ‘r’ on the keyboard.

Modifying the Plot

The appearance of an individual trace can be modified by placing the mouse over the trace and then double-clicking. This will display the Edit Trace window.



The **Line Style** box controls the appearance of the trace on the plot. The pattern, width and color of the line may be altered here.

The **Symbol Style** box controls the appearance of symbols on the plot. There is a symbol for each data point of a trace. In general it is not useful to display symbols for lines generated by the software, there will be too many of them and they will obscure the display.

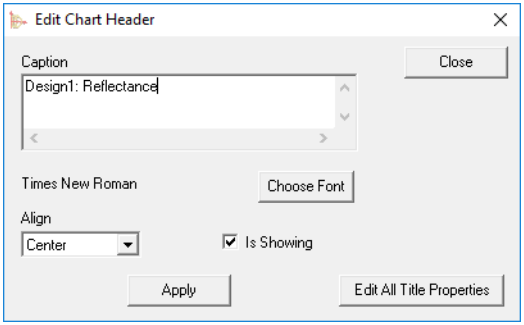
In the **Trace** box **Label** allows you to edit the text data displayed in the legend.

Selecting **Hidden** causes the trace to be removed from the display. If the axes are automatically scaled, then the data from the hidden trace will still be used in determining the scales. All hidden traces can be restored by selecting **Show all Hidden Traces** in the **Edit** menu of the plot.

Selecting **Excluded** causes the trace to be removed from the display and for automatically scaled axes excludes the data from being used to determine the scales. All excluded traces can be restored by selecting **Show all Excluded Traces** in the **Edit** menu of the plot.

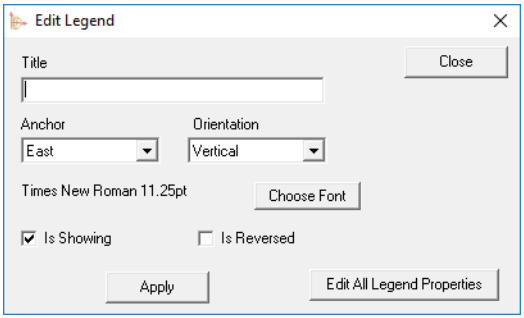
Selecting **Y2** causes the trace to be attached to the second axis, and selecting **Y1** causes it be attached to the first axis.

The plot title can be edited either by double-clicking on the title, or by right-clicking the mouse when it is in the plot and then selecting **Edit Header**. The following window is displayed:



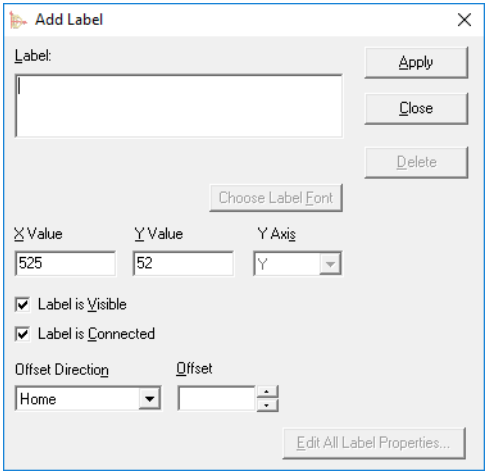
The plot can also have text at the bottom of the plot. This can be modified either by double-clicking on it or by right-clicking on the mouse when it is in the plot area and then selecting **Edit Footer**. A window similar to the **Edit Header** window will appear.

A plot may also have a legend. The legend provides extra textual information about each trace on the plot. The appearance of the legend may be controlled by either double-clicking on the legend, or by right-clicking the mouse when it is in the plot area and selecting **Edit Legend** from the menu that appears.



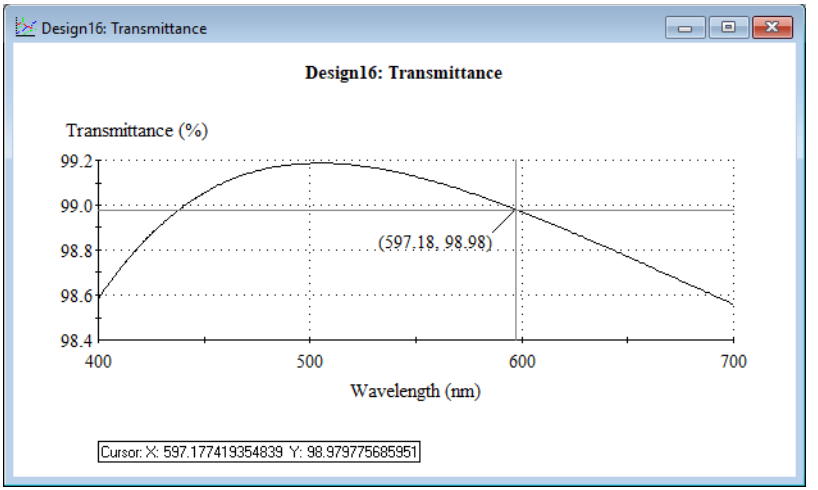
A title can be given to the legend. The position and layout of the legend are controlled by the **Anchor** and **Orientation** settings.

Labels can be added to the plot in two ways : A label can be added by moving the mouse to the location in the plot area where the label is to appear, then right-clicking will display the context menu. Selecting **Add Label…** will show the Add Label dialog.



The Add Label dialog allows you to enter the text to be displayed in the Label box, adjust the x and y location and control the label position with respect to the x and y location. The x and y location are given in terms of the plot's axes. If the plot has two Y axes, then the **Y Axis** drop down list can be used to choose the Y axis to which the Y value refers. The label position is controlled by **Offset Direction** and **Offset**. **Offset Direction** controls the direction in which the label is moved and **Offset** controls the distance. If **Label is Connected** is checked, a line is drawn from the label to the x,y location. Click the **Apply** button to add the label to the plot. Once the label has been added to the plot, you will be able to change the font.

When the plot cursor is active, you can also right-click in the plot and select **Add Cursor as Label…** This will add a label to the plot showing the current cursor co-ordinates.

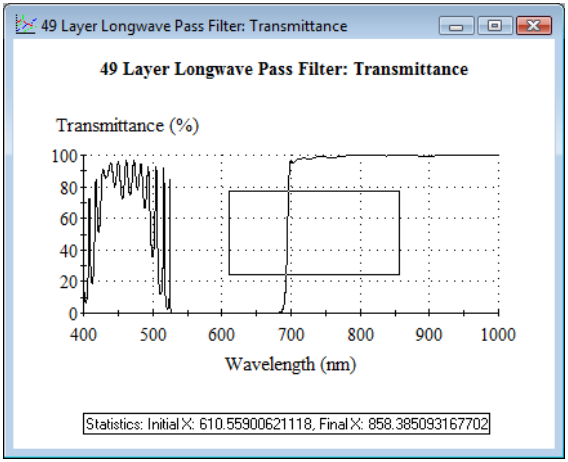


Labels can also be edited once they have been added to the plot. To edit a label, double-click on the label. The Edit Label dialog will appear. It has the same appearance as the Add Label dialog.

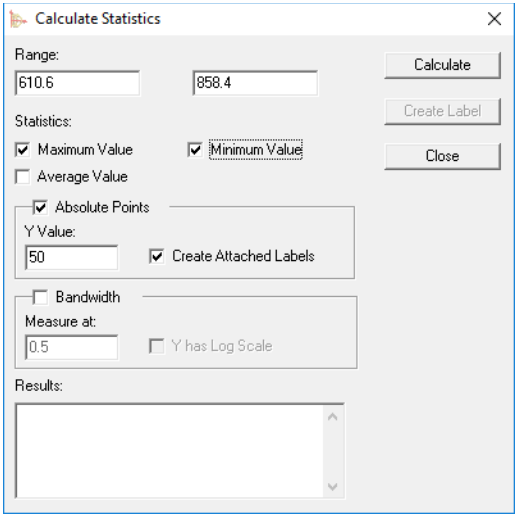
The position of a label can also be changed by dragging it on the plot. To drag, move the mouse over the label and then hold the left mouse whilst moving the label to the desired position. For labels that have an Offset Direction of Home, the label can be dragged anywhere in the plot area. For other labels, the label is restricted to lie along one of eight compass directions (North, South, East, West, Northeast, Southeast, Northwest, Southwest) from the point that it is labeling, but the distance is continuously variable.

Statistics

Statistical properties of the traces displayed on the plot can be calculated by right-clicking on the plot and selecting the **Statistics** command. First the X-axis range over which the statistics will be calculated must be selected. To do this, move the mouse to one end of the desired range. As you move the mouse around the plot, the bottom of the plot will show the current x co-ordinate. When the mouse is in the correct position, drag the mouse using the left button to the other end of the desired range. As you are dragging the mouse, the bottom of the plot will show the current x co-ordinate. Also a rectangle will appear on the plot. The vertical sides of the rectangle show the current x axis range. The horizontal sides of the rectangle are not used by the statistics command. When the mouse is in the correct position, release the mouse button.



The Statistics dialog will now appear. The selected x range is shown at the top of the dialog. If the values are not correct or need some adjustment, you can change the values.



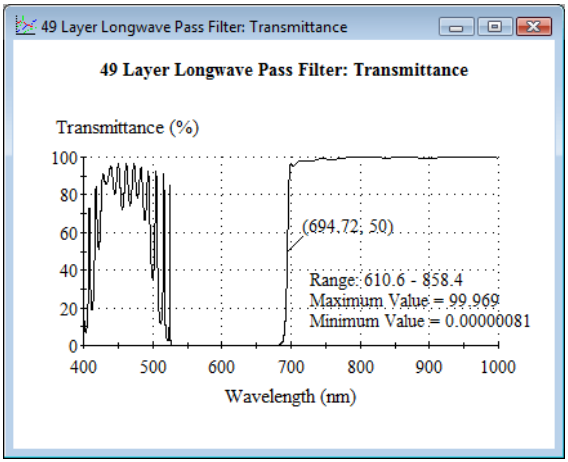
The statistics to be calculated are selected beneath the range dialog. **Maximum Value**, **Minimum Value** and **Average Value** calculate the maximum Y value, minimum Y value and mean Y value respectively over the X range for each trace on the plot.

Absolute Points will find all the locations on each trace where the trace has the value **Y Value**. If **Create Attached Labels** is checked, each absolute point will be marked with a label showing the co-ordinate of that point; otherwise each x-axis value will appear in the statistics results.

Bandwidth will calculate the bandwidth of a pass-band region on the plot. The Y value at which the bandwidth is calculated is a function of the **Measure At** value. When **Y**

has Log Scale is not checked, the Y Value is calculated by multiplying the maximum Y value in the range by the **Measure At** value. Thus, to calculate the FWHM value, the **Measure At** value should be 0.5. When **Y has Log Value** is checked, the Y value is given by the difference between the maximum Y value and the **Measure At** value. So to calculate FWHM on a log plot where the Y axis is in dB units, the **Measure At** value should be -3 (the sign of the **Measure At** number is ignored).

Once the desired statistics options have been set, click **Calculate** to generate the statistics. If **Absolute Points** has been selected and **Create Attached Labels** has been selected, the absolute point labels will appear on the plot. The results of the other statistics calculations will appear in the **Results** box. The information in this box can be edited. Click the **Create Label** button to add the contents of the box to the plot. The information will placed in the top right corner of the plot, but can be dragged to any other location after the Statistics dialog has been closed.



File Menu (Plot)

The Plot Window File Menu is similar to the Design Window File Menu except that there are three additional items, **Add Line...**, **Add Point...**. and **Export**.

Add Line...

This command is used to add to the plot a further curve derived from an existing plot or a table column. The plot or table must be already saved in a plot or table file. Selection of the command presents a dialog box for selection of the file for plotting. If a plot file is concerned the program will then plot the curve or curves over the existing one. If a table is chosen then it will first be presented for selection of the particular column. (See **Plot Column** below for more information). The plot derived from a table will always first be presented with symbols to mark the points. An alternative to the Add Line command is to drag and drop a plot from one window to another. In this case, neither plot needs to have been saved beforehand.

Add Point...

Add Point... is similar to **Add Line** but the file to be selected is a table file that contains a set of single values (chromaticity coordinates for example). The program assumes that the first two points are, respectively, the horizontal (independent) coordinate and the vertical (dependent) coordinate. These define a point that is plotted provided it lies within the axes. Should the table file have several columns, the column selection box will be presented. The point will then take the first value and second value in the column and plot the corresponding point. The principal use of this procedure is in plotting single results from the Function Enhancement such as chromaticity coordinates.

Export

Export has a sub-menu with two entries **Tab separated text** and **Comma separated values**. Both of these options create files containing the data shown in the plot, The Tab separated plot form uses a tab character in between the values and the Comma separated value form uses a comma to separate the values. The comma separated value form is best used when the data are to be imported into a spreadsheet.

Edit Menu (Plot)

Parameters...

The **Parameters...** menu item presents a dialog box that applies to the active plot. This dialog provides control over the presentation of the plot. Many aspects of the plot may be modified. A help system is provided to guide you through the various options. Any changes made to the plot do not alter the data corresponding to the plot. There is no recalculation. For instance if the horizontal axis corresponds to incident angle then even though the title of the axis is changed to wavelength, the data will still refer to incident angle and the plot will not change. If the values along the axes are changed then the data will be replotted according to the new values. Again it will not be recalculated. If data does not exist corresponding to some of the values then that part of the plot will be missing.

Copy

This command, as it does with other windows, copies the contents of the window to the clipboard from which it can be pasted into any other application. Note that what is stored on the clipboard is the plot itself and not the data. The plot file produced by the program stores the actual data used to create the plot.

One to One Aspect Ratio

One to One Aspect Ratio is used only in plots where it is important to have the axes with the same scale factor. These are primarily in some of the Analysis tools where it is important that circles should remain circles and not be converted to ellipses. In the bulk of the core Essential Macleod the checking of the box has no effect.

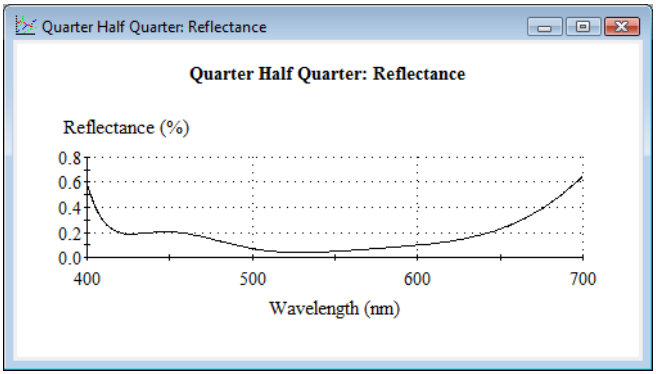
Clear Cursor

If the cursor has been enabled by holding down the **<Alt>** and dragging the mouse with the left button pressed, then selecting this command will remove the cursor from the plot.

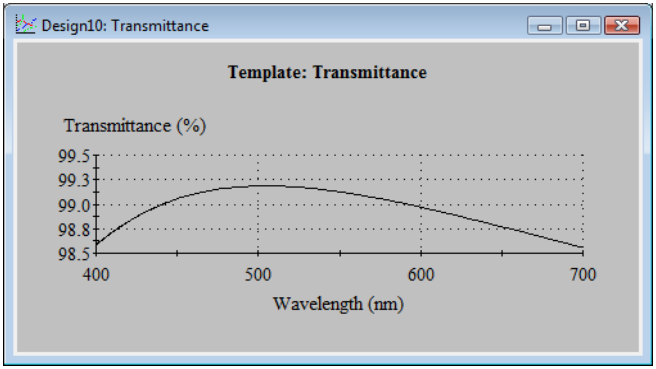
Apply Template...

This command applies the background and font parameters of a previously saved plot to the current plot without affecting the data in the plot.

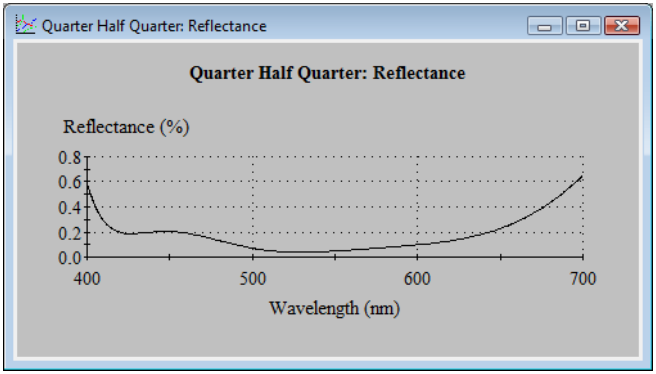
For example, the picture below shows a reflectance plot from a Quarter-Half-Quarter AR design.



The next picture shows a saved plot with modified background and title font.



The final picture shows the result of applying the template to the QHQ plot.



Identify Y Axes

Selecting this menu option will cause the y axes to be identified using the identifiers defined on the Plotting tab of the General Options window (from the Options menu, select General)

Unidentify Y Axes.

Selecting this menu option will cause any recognized axis identifiers to be removed from the Y-axis titles and from the legend

3D PLOT WINDOW

3D plots are shown in a 3D Plot window. Several of these may be open at any one time. They may also be reduced to icons by using the minimize button.

When the plot window is active you can hold down the **<Alt>** key and use the left mouse button to display x -, y- and z- coordinates of the nearest point on the plotted surface to the current cursor position. If you wish to remove the co-ordinate display, click **Clear Cursor** in the Edit menu, or right –click on the mouse when it is over the plot and select **Clear Cursor** from the menu that appears.

Plot Rotate

To rotate the plot, hold both mouse buttons down (or the middle button on a 3-button mouse) and move the mouse in the desired direction. The rotation can be constrained to be about a particular axis by holding down the x or y or z or e key and then moving the mouse perpendicular to the axis.

Plot Translate

The position of the plot in the window can be moved by holding down the **<Shift**> key, holding down both mouse buttons down (or the middle button on a 3-button mouse) and moving the mouse to the new location. To reset the position of the plot back to its default location, press the ‘r’ key on the keyboard.

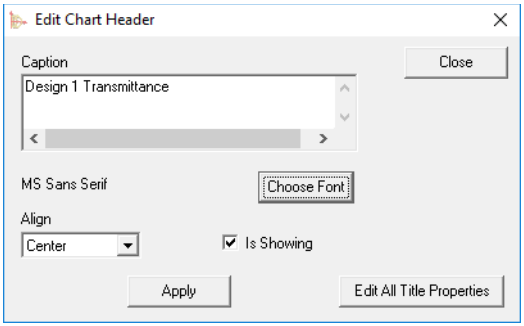
Plot Scale

The size of the plot in the window can be changed by holding down the **<Ctrl>** key, holding down both mouse buttons down (or the middle button on a 3-button mouse) and moving the mouse down to increase the chart size or up to decrease the chart size. To reset the position of the plot back to its default location, press the ‘r’ key on the keyboard.

Plot Zoom

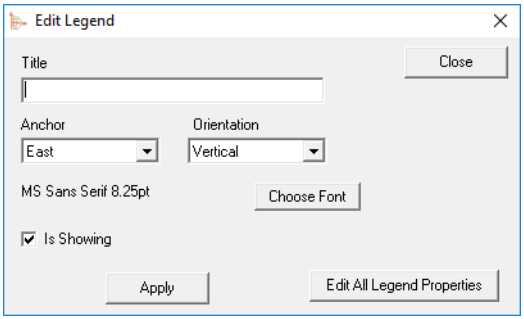
To zoom in to a particular area of a plot, hold the **<Ctrl>** down and whilst holding down the left mouse button, drag the mouse to define the zoom area. When you release the left mouse button, the plot will be redrawn so that the zoom area fills the plot. To reset the plot so that it shows all the data, press the letter ‘r’ on the keyboard.

The plot title can be edited either by double-clicking on the title, or by right-clicking the mouse when it is in the plot and then selecting **Edit Header**. The following window is displayed:



The plot can also have text at the bottom of the plot. This can be modified either by double-clicking on it or by right-clicking on the mouse when it is in the plot area and then selecting **Edit Footer**. A window similar to the **Edit Header** window will appear.

A plot may also have a legend. The legend provides extra textual information about each trace on the plot. The appearance of the legend may be controlled by either double-clicking on the legend, or by right-clicking the mouse when it is in the plot area and selecting **Edit Legend** from the menu that appears.



A title can be given to the legend. The position and layout of the legend are controlled by the **Anchor** and **Orientation** settings.

File Menu (3D Plot)

The 3D Plot Window File Menu is similar to the Design Window File Menu except that there is an additional item, **Export**.

Export

Export has a sub-menu with two entries **Tab separated text** and **Comma separated values**. Both of these options create files containing the data shown in the plot, The Tab separated plot form uses a tab character in between the values and the Comma separated value form uses a comma to separate the values. The comma separated value form is best used when the data are to be imported into a spreadsheet.

Edit Menu (3D Plot)

Parameters...

The **Parameters...** menu item presents a dialog box that applies to the active plot. This dialog provides control over the presentation of the plot. Many aspects of the plot may be modified. A help system is provided to guide you through the various options. Any changes made to the plot do not alter the data corresponding to the plot. There is no recalculation. For instance if the horizontal axis corresponds to incident angle then even though the title of the axis is changed to wavelength, the data will still refer to incident angle and the plot will not change. If the values along the axes are changed then the data will be replotted according to the new values. Again it will not be recalculated. If data does not exist corresponding to some of the values then that part of the plot will be missing.

Copy

This command, as it does with other windows, copies the contents of the window to the clipboard from which it can be pasted into any other application. Note that what is stored on the clipboard is the plot itself and not the data. The plot file produced by the program stores the actual data used to create the plot.

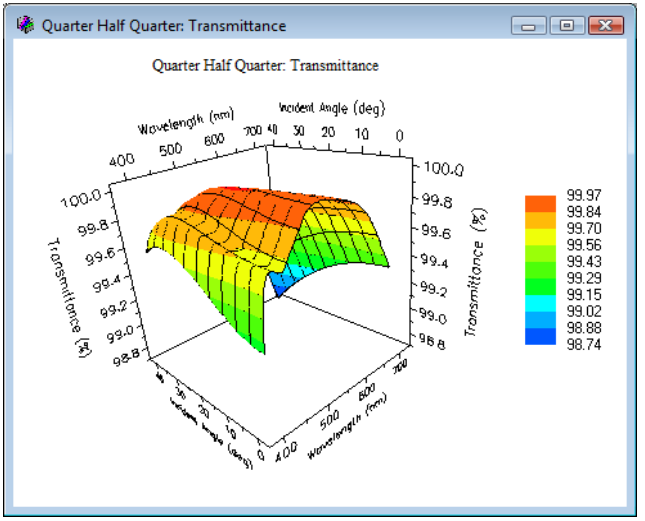
Clear Cursor

If the co-ordinate display has been enabled by holding down the **<Alt>** and dragging the mouse with the left button pressed, then selecting this command will remove the co-ordinate display from the plot.

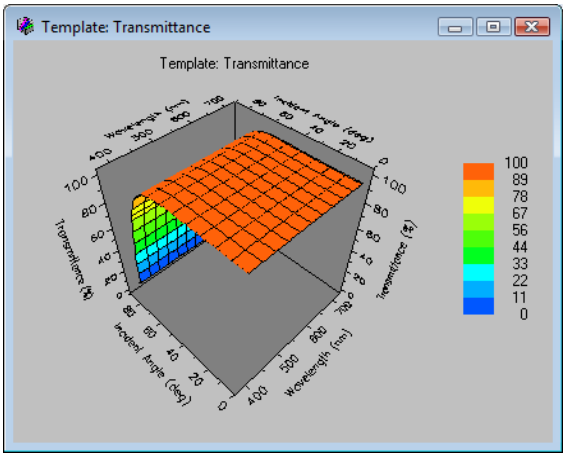
Apply Template...

This command applies the background and font parameters of a previously saved plot to the current plot without affecting the data in the plot.

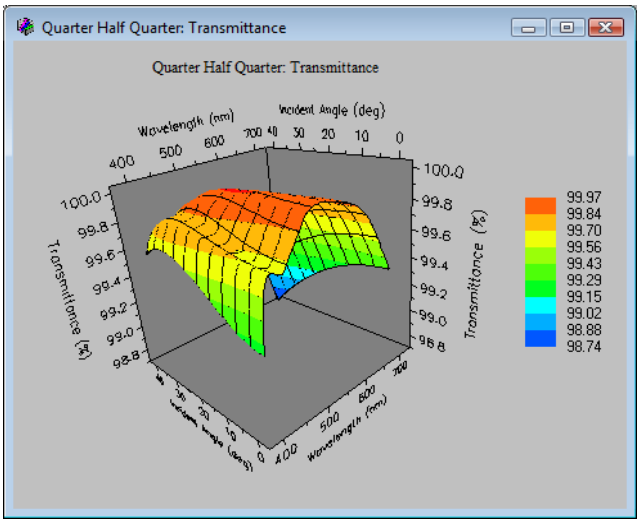
For example, the picture below shows a reflectance plot from a Quarter-Half-Quarter AR design.



The next picture shows a saved plot with modified background and title font.



The final picture shows the result of applying the template to the QHQ plot.



ACTIVE PLOT WINDOW

The Active Plot window is an extension of the capabilities of the Plot window. It is available for performance and analysis parameters of Designs. The Active Plot window allows you to immediately observe the effects of changing parameters of the design. To use the Active Plot, you first add variables to the Active Plot window. These represent the Design parameters that you wish to be able to change. You can then use the buttons associated with each variable to adjust the value of the variable. The plot will be updated each time a variable changes value. The Active Plot allows you to save the current Design back into the design window or copy it to the clipboard. You can also freeze the current plot. This means that the next time a variable changes value a new set of curves will be drawn on the plot rather than changing the existing curves.

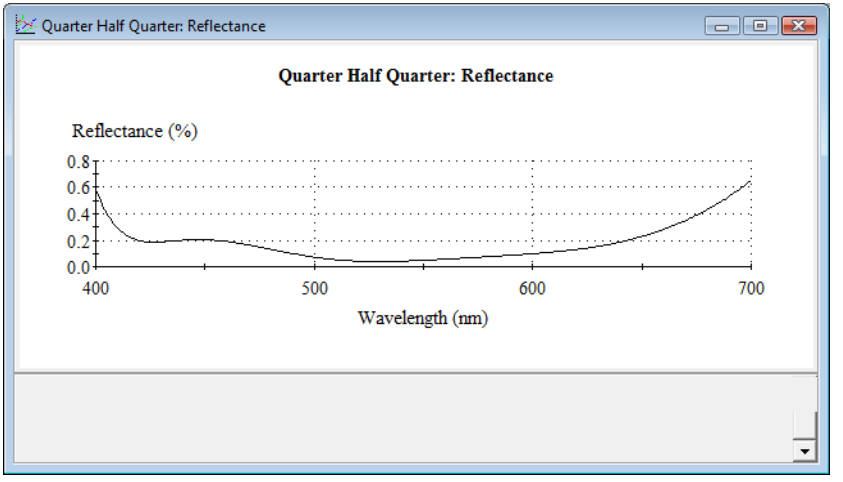
Start Active Plot by clicking the Active Plot button. The Active Plot button is located on the Performance dialog in the Parameters menu of the Design window and the Analysis parameters dialogs in the Analysis sub-menu of the Tools menu of the Design window. You can also start an Active Plot from the Performance menu of the Design window.

Active Plot supports multiple plot windows. Starting another Active Plot will create another Active Plot window. This window does not include the variables. Changing the variables in the first Active Plot window will update the additional Active Plot windows as well as the first Plot Window.

The additional capabilities of the Active Plot window are described below. The Active Plot window also supports the capabilities of the Plot window. See the Plot Window chapter for more information on the Plot window capabilities.

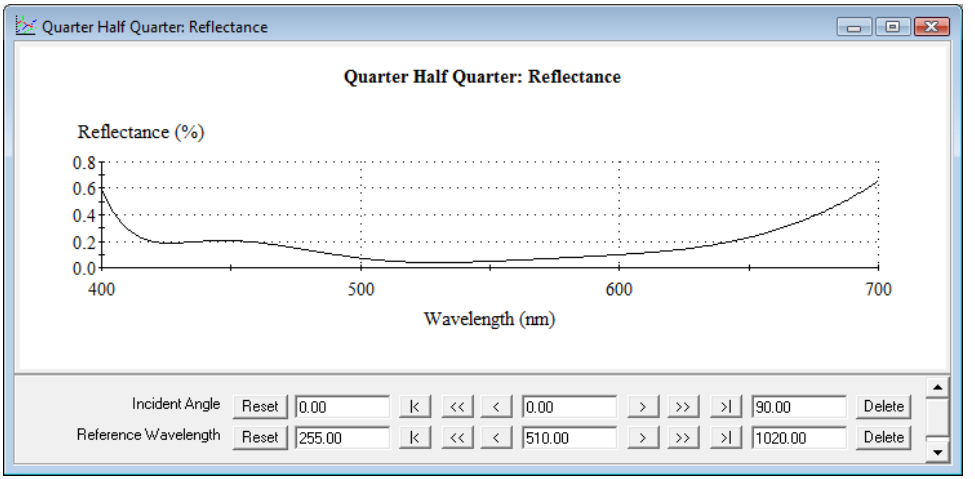
Active Plot Display

There are two sections to the Active Plot display. The top section contains the plot and the bottom section contains the variables. When the Active Plot is opened for the first time for a design, the bottom section is empty.



The Active Plot window has two extra menu items when compared to the Plot window. These are the **Add** menu and the **Active** Menu.

Variables are added to the window by selecting items from the Add menu (the Add menu is described in detail below). The figure below shows the Active Plot window after Incident Angle and Reference Wavelength variables have been added.



For each variable added, a row is created in the bottom section of the window. The row contains several buttons and three text boxes. The left box shows the lower limit of the variable. The center box shows the current value of the variable. The right box shows the upper limit of the variable. The buttons provide the following actions:

|< Moves the current value to the lower limit

<< Moves the current value towards the lower limit by 10% of the difference between the limits (Fast Down).

< Moves the current value towards the lower limit by 1% of the difference between the limits (Down).

> Moves the current value towards the upper limit by 1% of the difference between the limits (Up).

>> Moves the current value towards the upper limit by 10% of the difference between the limits (Fast Up).

>| Moves the current value to the upper limit

Reset Changes the current value to the value that is in the design.

Delete Removes the variable.

After the current value of a variable has been changed, the plot will be updated to reflect the new performance. Note that changing the values of variables does not affect

the design in the Design window. The design is only modified when the **Update Design** command in the Active menu is selected (see below).

You can change the values of the limits and the current value by typing in new values. When changing the current value, press **<Enter>** or click outside of the current value box, to update the plot.

To change the size of the bottom section, move the cursor to the line between the two sections. The cursor will to a double-headed arrow. Now click and drag the line to the desired position.

Add Menu

This menu contains all the options for adding variables to the Active Plot window. Variables are always added to the end of the existing variables.

Incident Angle

Adds Incident Angle. As this variable is changed, the incident angle of the plot calculation will be changed.

Reference Wavelength

Adds Reference Wavelength. As this variable is changed, the reference wavelength of the design will be changed.

Calculation Wavelength

Adds Calculation Wavelength. As this variable is changed, the calculation wavelength of the plot calculation will be changed.

Selected Layer Thicknesses

This command will add a layer thickness variable for each selected layer in the Design. You do not have to have selected the layers before opening the Active Plot. You can go back to the Design window and change the selection before using this command. You can also use this command several times to add different groups of layers.

All Layer Thicknesses

This command will add a layer thickness variable for each layer in the Design.

Selected Layer Packing Densities

This command will add a layer packing density variable for each selected layer in the Design. You do not have to have selected the layers before opening the Active Plot. You can go back to the Design window and change the selection before using this command. You can also use this command several times to add different groups of layers.

All Layer Packing Densities

This command will add a layer packing density variable for each layer in the Design.

Selected Layer Void Densities

This command will add a layer void density variable for each selected layer in the Design. You do not have to have selected the layers before opening the Active Plot. You

can go back to the Design window and change the selection before using this command. You can also use this command several times to add different groups of layers.

All Layer Void Densities

This command will add a layer void density variable for each layer in the Design.

Selected Layer Links

This command will add a link variable for each selected layer in the Design. You do not have to have selected the layers before opening the Active Plot. You can go back to the Design window and change the selection before using this command. You can also use this command several times to add different groups of layers. Each link is only added once to the variable list, even though the link may have selected many times. This variable operates by multiplying the thicknesses of all the layers in the link by the current value. This is useful for examining, for example, the effect of tooling factor changes on a design's performance.

All Layer Links

This command will add a link variable for each link in the Design.

Selected Layer Material Densities

This command will add a material packing density variable for each different material used in the selected layers of the Design. You do not have to have selected the layers before opening the Active Plot. You can go back to the Design window and change the selection before using this command. This variable operates by multiplying the packing densities of all layers using the material by the current value. This is useful for examining, for example, the effect of refractive index changes on a design's performance.

All Layer Material Densities

This command will add a material packing density variable for each different material used in the Design.

Selected Layer Void Material Densities

This command will add a material void density variable for each different material used in the selected layers of the Design. You do not have to have selected the layers before opening the Active Plot. You can go back to the Design window and change the selection before using this command. This variable operates by multiplying the packing densities of all layers using the material by the current value. This is useful for examining, for example, the effect of refractive index changes on a design's performance.

All Layer Void Material Densities

This command will add a material void density variable for each different material used in the Design.

Taper Distance

This command will add a taper distance variable. This is used to show how the design performance will change with uniformity errors. See the uniformity model (Page 24) for more information.

Active Menu

Freeze

The Freeze command saves the current plot curves and starts a new set of curves the next time a variable changes value.

Update Design

This command updates the design in the Design window with the design that has the performance shown in the Active Plot window.

Copy Design

This command copies the design that has the performance shown in the Active Plot window to the clipboard.

TABLE WINDOW

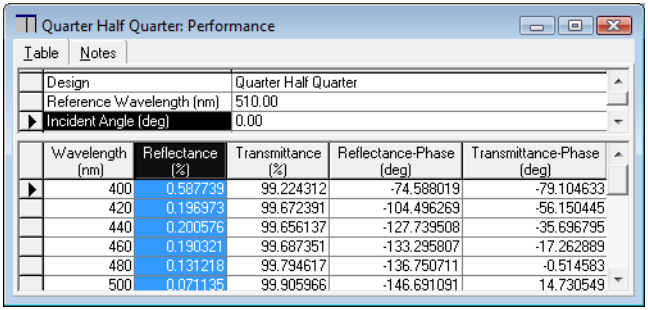
The Table Window displays the results of a calculation in tabular form. The tables result from selection of the Table command in the **Performance** menu of the Design Window. By clicking on the Notes tab, you can add other textual information that will be stored with the table. Most of the menu items are ones that are already familiar. Some deserve further explanation.

File Menu (Table)

The File Menu is similar to that for the Design Window but there is one extra item, **Plot Column**.

Plot Column

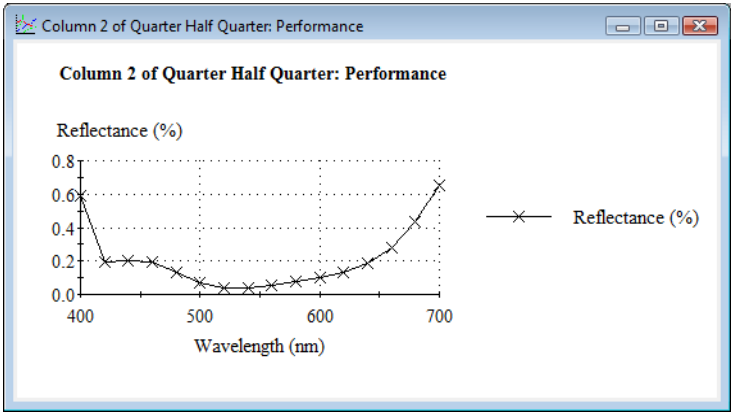
Plot Column activates the plotting of results from a column in the table that is active. Select the column that is to be plotted by clicking in the header of the column, then select Plot Column from the File menu.



The major difference between the plot produced from a table and a corresponding plot produced directly from a design is that the table interval may not be completely suitable. For example, fringes may be missed. To emphasize this the table data points are marked with crosses in the plot.

At this stage the axes have been automatically assigned scales that correspond to the extent of the data. The plot is in a normal plot window with the normal plot window menu.

Data from tables can be added to existing plots also by use of the **Add** command under the **File** menu when the plot window is active. For this operation the table must first have been saved as a table file.



A column of a table can also be added to a plot by using drag and drop. First, select the column to be added to a plot by clicking in the header for the column as for Plot Column. Next, move the cursor into the data of the selected column and drag to the plot that is to have the plotted data. When the cursor is inside the plot, release the mouse button to drop the column onto the plot.

Edit Menu (Table)

The **Edit Menu** is similar in most respects to other Edit Menus in the package. Commands that are significantly different either in name and/or function are listed below with a description of their action.

Copy Table

Copy Table places the table data onto the clipboard. Note that the data is held on the clipboard as tabular data and the format will depend on the nature of the application into which the results are pasted.

Read Only

Tables represent data that have been calculated and so there is a presumption that the data in a table are a true representation of performance as calculated. Editing of the table entries is something that should be entered into with extreme caution. The tables as they are generated are, therefore, arranged to be *read only* to discourage casual alteration. However, it may be necessary actually to alter some of the entries. This menu item permits the toggling of the *read only* status of the file. When a table is created by the New command the *read only* status is not set until the table is saved for the first time.

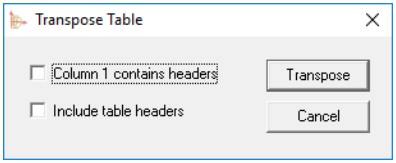
Sort Ascending

Sort Descending

These commands sort the table rows into ascending or descending order for the selected column. This is especially useful for importing data where, for example, wavelength data is in descending order, and ascending order is required. To perform the sort, select a column by clicking in the column header and then select the appropriate command from the Edit menu.

Transpose...

Sometimes the contents of a table of imported data might have the data arranged in rows instead of columns. The **Transpose** command can be use to swap the rows and columns. Selecting **Transpose** presents the following dialog box.



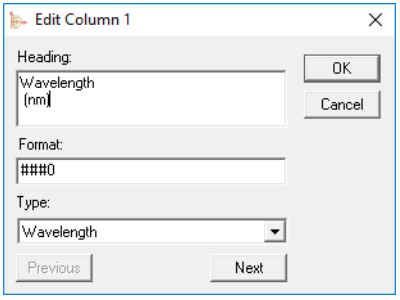
Checking **Column 1 contains headers** will cause the data in the leftmost column to become the column header in the transposed table. Checking **Include table headers** will cause the column header data to be placed in column 1 of the transposed table. Both options cannot be selected at the same time.

Columns...

This menu item presents a dialog box where the nature of the data to be stored in each column may be specified. The *read only* status will determine whether or not any changes will be implemented. Do check it first.

Three entries are required for each column.

The first is the column heading. This can be any suitable text expression.



The second is the column format. If the format is empty then the number or text is displayed without any formatting. For numbers, the format uses 0 (zero), #, ., E -, +. The 0 (zero) indicates a digit position where either a digit will be displayed, or if there is no digit in the number, a zero will be displayed, while # indicates a position where a digit will be displayed only if there is a corresponding one in the number. As usual the E indicates scientific number formatting. The E must be followed by a + or – symbol. A following - indicates that negative exponents will be displayed with a minus sign, while positive exponents will be displayed with no sign. The + indicates that all exponents will be displayed with an appropriate sign. For example the number 43.568434 is displayed as follows for each of the example formats:

Format	Displayed Number
##0.0000	43.5684
000.0000	043.5684
0.000E-000	4.357E001

Text strings are formatted using the @ character. The number of @ characters in the format determines the number of characters displayed. For example with a format of @, the string DEF is displayed as D and with a format of @@@ it is displayed as DEF

The third entry is the type of the data. Particularly in the full Essential Macleod package, the data must sometimes be of a specific type in order to be recognized elsewhere in the package. Tooling factors in Runsheet are examples. Available types are given in a scrolling list. The type "Unknown" is included.

There are two buttons, **Previous** and **Next** that transfer the editing to the columns on either side of the current one. Either button may be grayed out if the current column is at the limit of the table.

Once the table has been completed and saved it will be designated Read Only and that status must be changed in the **Edit** menu if any reediting is to be carried out.

The entry Format Syntax in on-line Help gives details of the various methods that may be used to define the format. Look up **Format Syntax** in **Search for Help on...** in the **Help** menu.

Tools Menu (Table)

The **Tools Menu** is similar in most respects to other Tool Menus in the package. This menu contains one item that is unique to tables.

Color

Color calculates the color co-ordinates of the selected column. The column is assumed to contain a transmission or reflection spectrum and the leftmost column is assumed to contain the wavelength points for the spectrum. The wavelength data must be in nanometres. To use this function, select the column that contains the data for which color is to be calculated. The leftmost column is assumed to contain the wavelength data. Select Color from the Tools menu. A simpler version of the Color parameters window will appear. This allows you to select the parameters for the color co-ordinates to be calculated. Click Plot to produce a plot and click Table for a table of data.

REFINEMENT AND SYNTHESIS

Refinement and synthesis are automatic processes for the improvement of design performance. They are quite similar in their operation. Refinement essentially implies improvement by application of, usually slight, modifications to an already existing starting design and synthesis involves an element of construction, which in extreme form can operate with virtually no starting design whatsoever.

To permit automatic assessment of improvement, an objective measure of performance is required which must be a single number. This is known as the figure of merit. The derivation of a figure of merit requires first of all that a target performance be defined. Then the actual performance is compared with the targets and the gap between actual and required performances is expressed by the function of merit as a single number. The function of merit is simply a set of rules that governs the conversion of the performance gap into a single figure. This may be accomplished in many different ways. In the Essential Macleod the target performance consists of a series of independent requirements known as targets. These might be the reflectance at a particular wavelength, the Group Delay Dispersion at another, or the ellipsometric parameters at a third, or the chromaticity coordinates of the light reflected from the coating at normal incidence under illumination by an equal energy source, or combinations of these or any of the other calculable performance parameters. Polarization and angle of incidence may also be specified. The relative importance of each target can be indicated by an assigned weight. The conversion of the gap between actual and target into a component of the merit function involves taking the absolute difference between them and then raising it to a specified integer power and multiplying by the assigned weight. Some complications of the merit function involving target linking are possible and are described under Targets later in this manual.

Refinement techniques differ largely in the way in which they use the history of gradual improvement in the figure of merit to plan further improvements. Synthesis techniques add to efficient refinement the possibility of increasing the number of adjustable parameters, that is, complicating the design, once refinement has apparently reached an impasse. Refinement is then re-launched. The complicating process may be arranged to operate periodically. The way in which the design is complicated differentiates the various forms of synthesis.

The Essential Macleod provides eight distinct classes of technique for refinement and/or synthesis. Simplex, sometimes called Nonlinear Simplex to distinguish it from a linear programming technique with the same name, is a very fast refinement technique that makes for the nearest merit function minimum. It is very stable – there is virtually zero probability of making things worse – and so it is particularly suitable for the adjustment of an already useful design. Tuning the outer layers of an edge filter to assure good performance in the pass region is a good example of a task ideally suited for Simplex. The implementation of Simplex accommodates packing density as well as film thickness permitting refinement in terms of index as well as assisting in reverse engineering. Optimac is a technique that has been developed by Thin Film Center Inc. It is both a refinement and a synthesis technique, but it has great strength in synthesis where it is capable of building a design virtually from scratch. Conjugate Gradient and Quasi-Newton are two refinement techniques that make use of derivative information when

determining the next move. Simulated Annealing is an intermediate technique that has some attributes of synthesis and is rather more than refinement. It ranges widely over parameter space, avoiding shallow local minima. It does not add layers like Optimac but it has few constraints and it has no need of a good starting design. All it requires is a sequence of layer materials, a range of thicknesses and/or packing densities, and plenty of time. Needle Synthesis is a technique for adding layers to a design. Needle Synthesis determines where to insert new layers by calculating the derivative of the merit figure for a layer with zero thickness as it is moved throughout the existing layers. New layers (up to the number specified) are inserted at the points where the merit figure derivative has its most negative values. Conjugate Gradient refinement is then used to expand the newly inserted layers from their initial zero thickness values to some positive values. Conjugate Gradient refinement may also adjust the thicknesses of other layers if this results in an improvement of the design. Differential Evolution is an evolutionary algorithm for finding an optimal design. The Differential Evolution algorithm is discussed in "Differential Evolution A Practical Approach to Global Optimization" by Kenneth Price, Rainer M. Storm and Jouni Lampinen. Finally Non-Local Refinement attempts to find better designs by randomizing the starting point for refinement and calling the selected refinement method many times.

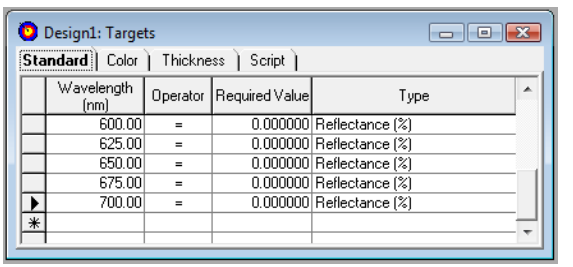
The various techniques share the same targets but there are also other attributes that must be set correctly for the processes to proceed and differ from one technique to the other. They are discussed under the Parameters heading.

For applications where the thickness of the layers must lie within some range, the upper and lower limits in physical thickness can be specified in the design in the Minimum Physical Thickness and Maximum Physical Thickness column.

Targets for refinement

Targets are grouped into four categories: Standard, Color, Thickness and Script (Script targets require the Function enhancement). All the Standard targets require a wavelength to be defined and include parameters such as Reflectance Magnitude, Transmittance Phase, Transmittance GDD and Reflectance Delta. The Color targets contain all the color parameters that may be used as targets. The Thickness targets allow total thicknesses for materials to be specified as targets. Script targets call functions written in the scripting language.

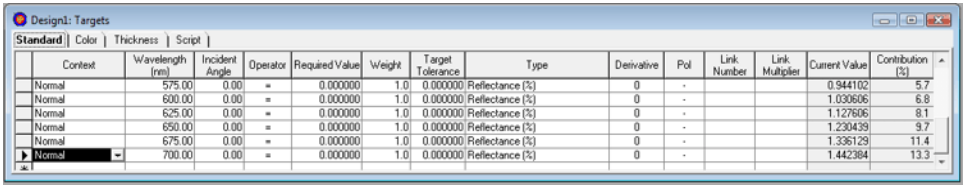
Standard Targets



A new refinement standard targets window contains only four columns, wavelength or frequency, operator, required value and type. Frequently these are all that is required. Other attributes of the targets are set to default values. Incident angle is zero, weights are all unity and tolerances have their default values. Targets may be either equality targets or inequality targets. This is specified by the operator.

The other target attributes can be activated by the menu item, **Display Setup >** in the **File** menu. The sub-menu that appears has the following entries, **Context**, **Incident Angle**, **Weight**, **Tolerance, Derivative**, **Link** and **Current Value**. Note that Context only appears for Design Targets.

Selecting all of these gives a window similar to the following.



Context	Wavelength (nm)	Incident Angle	Operator	Required Value	Weight	Target Tolerance	Type	Derivative	Pol	Link Number	Link Multiplier	Current Value	Contribution (%)
Normal	575.00	0.00	=	0.000000	1.0	0.000000	Reflectance (%)	0	-			0.944102	5.7
Normal	600.00	0.00	=	0.000000	1.0	0.000000	Reflectance (%)	0	-			1.030606	6.8
Normal	625.00	0.00	=	0.000000	1.0	0.000000	Reflectance (%)	0	-			1.127606	8.1
Normal	650.00	0.00	=	0.000000	1.0	0.000000	Reflectance (%)	0	-			1.230439	9.7
Normal	675.00	0.00	=	0.000000	1.0	0.000000	Reflectance (%)	0	-			1.336129	11.4
Normal	700.00	0.00	=	0.000000	1.0	0.000000	Reflectance (%)	0	-			1.442384	13.3

Context specifies the design context in which the target applies.

Incident Angle is measured in the current incident angle units and when the incident angle column is present the polarization column (Pol) is also automatically activated.

The **Weight** column controls the relative importance of each target. The larger the value of the weight of a target relative to others, the more the refinement will be driven by the performance at that target.

The **Target Tolerance** column indicates the relative acceptable error magnitude of each target. For each target, the difference between the required value and actual value is divided by the tolerance. When the Type of a target is changed, the default tolerance for the target type will be inserted in Target Tolerance column. The default tolerance values may be edited by selecting **Tolerances** from the **Options** menu.

The **Derivative** column lists the order of the derivative of the target type with respect to the independent variable that is either wavelength or frequency, whichever is listed in the first column. An order of zero indicates that no derivative is involved.

Link permits the assignment of relationships between targets. For example, it might be required that the reflectance at 525nm should be 4% greater than that at 550nm but that the absolute level of the reflectance be unimportant. To arrange this we first of all link the two targets together by giving each the identical link number, in this case unity. Note that as the link numbers are entered so the Required Value against the second linked target disappears and also that the number unity appears by default in the Link Multiplier column. Now we want the difference between the values to be 4% and so we set the multiplier for 550nm to -1 and the Required Value against 525nm to be 4%. By default the weight given to the combination is unity. It can be adjusted by forcing the appearance of the Weight column.

More than two values can be linked. The links are interpreted in this way.

$$Linked\ Value = \sum_{Link} (Link\ Multiplier\ \times Value\ of\ given\ Type)$$

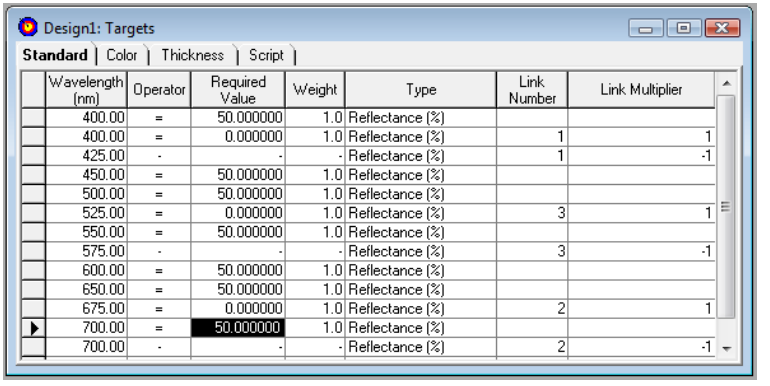
$$Merit\ function\ component = Weight\ \times\ |Required\ value\ -\ Linked\ Value|^{Power}$$

If all the types involved in a particular link are phases then the principal values of the phases will be used and the result will be expressed as the principal value. If only some of the values involved in a single link are phases (this may not make any physical sense) then the principal values of the individual phases will be derived but from then on the phases will be considered as simple numbers and the final result will be completely untreated.

As an example of a refinement operation that uses linking we can imagine that we want to derive a beam splitter coating with 50% reflectance at normal incidence over the region 400 to 700nm. We use ZnS and Na3AlF6 (cryolite) as materials on glass with air as incident medium. We use a starting design of nine layers of optical thickness 0.15 at 510nm with Na3AlF6 outermost.

We first set up a conventional set of targets, that is reflectance 50% from 400 to 700nm at intervals of 25nm. We use simplex with a starting thickness increment of 0.01. The simplex during the refinement process eliminates two layers to yield a seven-layer design with Na3AlF6 outermost and a performance given by the thinner line (red) in the following plot.

Next we construct a set of targets that consist of absolute values of 50% at 400, 450, 500, 550, 600, 650 and 700nm, but we add separate links of 400 with 425nm, 525 with 575nm and 675 with 700nm each requiring zero difference between the values of reflectance. The link multipliers, in other words, are set to 1 and -1. The weights are set at three, larger than the unity values for the individual targets, to emphasize the links. The arrangement is shown in the following table.

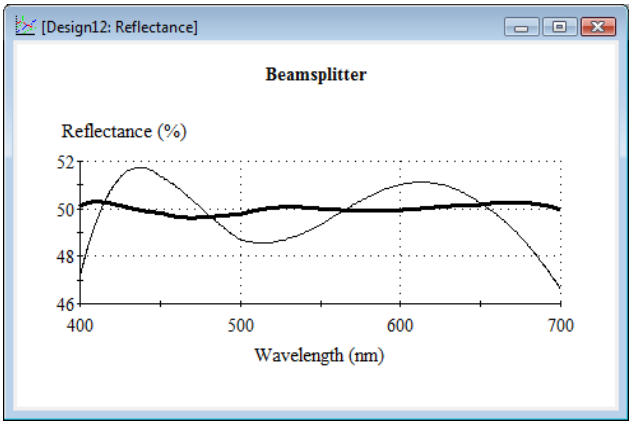


	Wavelength (nm)	Operator	Required Value	Weight	Type	Link Number	Link Multiplier
	400.00	=	50.000000	1.0	Reflectance (%)		
	400.00	=	0.000000	1.0	Reflectance (%)	1	1
	425.00	-	-	-	Reflectance (%)	1	-1
	450.00	=	50.000000	1.0	Reflectance (%)		
	500.00	=	50.000000	1.0	Reflectance (%)		
	525.00	=	0.000000	1.0	Reflectance (%)	3	1
	550.00	=	50.000000	1.0	Reflectance (%)		
	575.00	-	-	-	Reflectance (%)	3	-1
	600.00	=	50.000000	1.0	Reflectance (%)		
	650.00	=	50.000000	1.0	Reflectance (%)		
	675.00	=	0.000000	1.0	Reflectance (%)	2	1
▶	700.00	=	50.000000	1.0	Reflectance (%)		
	700.00	-	-	-	Reflectance (%)	2	-1

This maintains the nine layers of the design during the course of the simplex refinement with identical parameters and a much flatter performance is obtained. In the

plot below, the heavier line shows the performance of the design refined with linked targets.

Links give an added dimension to the refinement and synthesis specifications and increase greatly the power of the technique. However, a word of caution is appropriate. A performance specified with links can often be more difficult to achieve than one without, and so the convergence will take longer. It is also very easy to demand a completely unreasonable performance and in such a case the process will be very slow and the result disappointing.

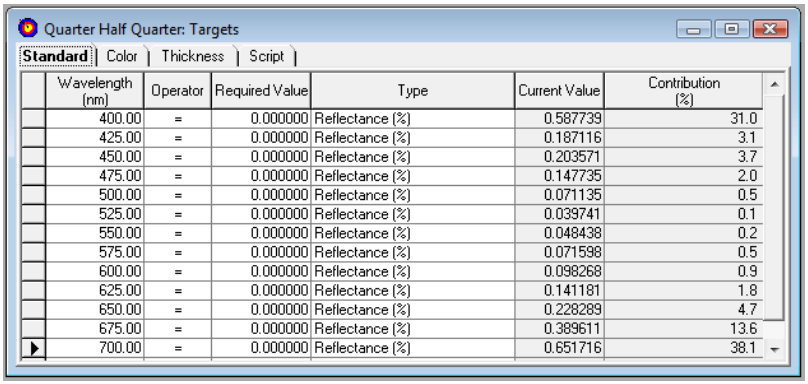


Links can also be used for calculating average values. Average value calculations are available for magnitude related targets. The link calculations are performed in the same way except that the final value is divided by the sum of the link multipliers. That is:

$$Average\ Value = \frac{\sum_{Link}(Link\ Multiplier\ \times Value\ of\ given\ Type)}{\sum_{Link}(Link\ Multiplier\ )}$$

An unweighted average will be calculated when all link multipliers have the same value. A weighted average can be calculated by setting the link multipliers to the desired weights. Note that the average calculation is only performed at the specific wavelengths in each set of linked targets. If there are significant excursions between the target points, more targets will need to be added to bring the calculated average value closer to the average value of the spectrum.

The **Current Value** and **Contribution** columns provide data on the performance of the design for the current set of targets.

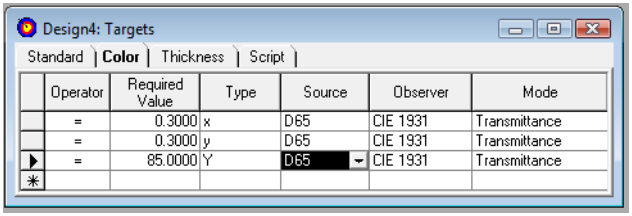


Wavelength (nm)	Operator	Required Value	Type	Current Value	Contribution (%)
400.00	=	0.000000	Reflectance (%)	0.587739	31.0
425.00	=	0.000000	Reflectance (%)	0.187116	3.1
450.00	=	0.000000	Reflectance (%)	0.203571	3.7
475.00	=	0.000000	Reflectance (%)	0.147735	2.0
500.00	=	0.000000	Reflectance (%)	0.071135	0.5
525.00	=	0.000000	Reflectance (%)	0.039741	0.1
550.00	=	0.000000	Reflectance (%)	0.048438	0.2
575.00	=	0.000000	Reflectance (%)	0.071598	0.5
600.00	=	0.000000	Reflectance (%)	0.098268	0.9
625.00	=	0.000000	Reflectance (%)	0.141181	1.8
650.00	=	0.000000	Reflectance (%)	0.228289	4.7
675.00	=	0.000000	Reflectance (%)	0.389611	13.6
700.00	=	0.000000	Reflectance (%)	0.651716	38.1

The Current Value column shows the actual design performance value for the target. The Contribution column shows the % contribution of the target to the total merit figure.

The principal menu item that concerns us when the target window is active is the **Edit** menu. The other items are the usual general ones concerning the package as a whole.

Color Targets



Operator	Required Value	Type	Source	Observer	Mode
=	0.3000	x	D65	CIE 1931	Transmittance
=	0.3000	y	D65	CIE 1931	Transmittance
=	85.0000	Y	D65	CIE 1931	Transmittance

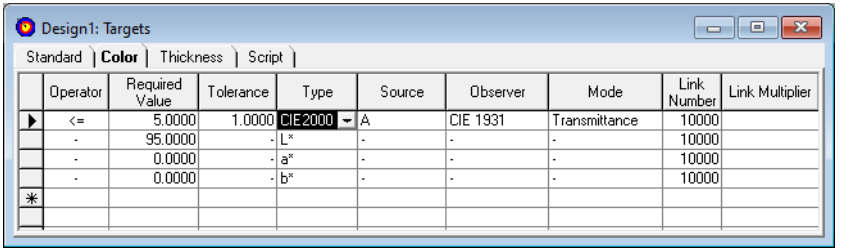
A color targets window contains different columns to the standard targets window. Required Value, Type and Operator have the same meaning as for the standard targets except that types are all color parameters. Each target also specifies a source distribution, and an observer. The mode specifies whether transmitted or reflected color is to be calculated. For stacks, an additional mode is Back Reflectance. This calculates the reflected color from the emergent medium side of the stack. For vStacks, only throughput is available for the Mode. To avoid taking too much screen space, the target types have been abbreviated as follows:

X	Tristimulus X
Y	Tristimulus Y
Z	Tristimulus Z
x	Chromaticity x
y	Chromaticity y

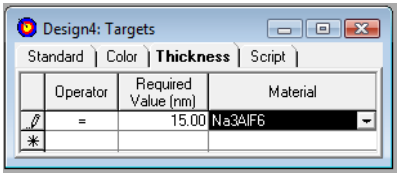
z	Chromaticity z
L*	CIE 1976 L*
a*	CIE 1976 a*
b*	CIE 1976 b*
u*	CIE 1976 u*
v*	CIE 1976 v*
u’	CIE 1976 u’
v’	CIE 1976 v’
c*(ab)	CIE 1976 chroma correlate of L*a*b*
h*(ab)	CIE 1976 hue correlate of L*a*b*
c*(uv)	CIE 1976 chroma correlate of L*u*v*
h*(uv)	CIE 1976 hue correlate of L*u*v*
s*(uv)	CIE 1976 saturation correlate of L*u*v*
CIE2000	CIEDE2000 color difference
CIE76	CIE76 color difference
L	Hunter L
A	Hunter A
B	Hunter B
u	CIE 1960 u
v	CIE 1960 v
CCT(K)	Correlated Color Temperature (Kelvin)
RCCT(RMK)	Reciprocal Correlated Color Temperature (Reciprocal Mega Kelvin)
Wd	Dominant Wavelength
Wc	Complementary Wavelength
Pe	Excitation Purity
Pc	Colorimetric Purity
Ra	General Color Rendering Index
R1 – R14	Specific Color Rendering Index
DC	Chromaticity Difference

Other color target attributes such as Incident Angle, Weight, Tolerance, Link and Current Value may be displayed by using the **Display Setup** command in the **File** menu. These attributes have the same meanings as for standard targets. The Display Setup command applies to all of the different target windows, but only the columns appropriate for the window are displayed.

The color difference targets (CIE2000, CIE76) require reference L*a*b* or L*c*h* color coordinates for the calculation. These color coordinates are attached to the color difference by using the same link number for each target. For convenience, when adding a color difference target, reference color coordinates will be automatically added by the program with a unique link number. The figure below shows a single color difference target with its associated reference color coordinates.



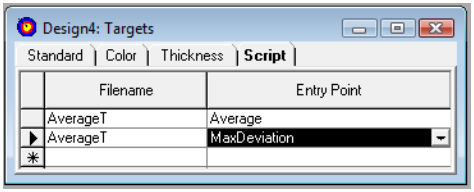
Thickness Targets



The thickness targets window normally only shows the material, operator and the desired total thickness of the material. When one or more total thickness targets are present, refinement will attempt to move the total thicknesses of the materials to the required values at the same time as attempting to meet the other targets. Thickness targets are only available for designs.

Other columns that are controlled by the **Display Setup** command that apply to the thickness target window are Weight, Tolerance, Link and Current Value. These columns have the same meaning as for standard targets.

Script Targets



The script targets window normally only shows the filename, and entry point columns. During the evaluation of a design, each script target is calculated by calling the entry point in the filename. The entry point returns a number indicating how well the design meets the requirement expressed by the script target. The result of the entry point corresponds to the portion of the merit function that computes:

$$\frac{|Required\ Value - Actual\ Value|}{Tolerance}$$

The Required Value and Tolerance are to be provided by the script and do not appear in the Script Targets table. The result is combined with the other target results in the same using the Merit Function Power and Weight. Detailed information on script targets is provided in the Scripting Language Help in the online Help system.

Script targets are only available for designs and can only be used with Simplex, Optimac and Simulated Annealing refinement. The Function enhancement is required to use Script Targets.

The Weight and Current Value columns are controlled by the **Display Setup** command.. These columns have the same meaning as for standard targets.

Edit Menu (Targets)

Some of the items in the menu may not be available until the corresponding parameters in the targets window are selected.

To select a row in the window, place the cursor over the small selection box on the extreme left and click once to select the box and a second time to select the row. To select a block of rows, select the first and then with the shift key depressed select the last. To deselect a block, place the cursor on any of the selection boxes and click once.

Cut Rows

Once rows are selected in the same manner as rows in the design window then they can be cut from the targets and placed on the clipboard.

Copy Targets

Copy targets copies all of the targets and stores them on the clipboard so that they can be pasted into another design. If you copy the targets and then paste them back into the

current design no change will be observed. Use **Copy Rows** and **Paste Rows** to duplicate parts of the current targets.

Copy Rows

Copies the selected rows onto the clipboard.

Paste Targets

Pastes the set of targets stored on the clipboard to the current target window. This operation replaces the current set of targets.

If the target data was placed on the clipboard by an application other than the Essential Macleod, then the Import Data tool (See page 44) will be used so that you can specify which columns on the clipboard correspond to the various target window columns. Additionally you can specify every n'th line is read. This is typically used to reduce the number of target points when the data on the clipboard is the output of a spectrometer scan.

Paste Rows

Pastes the rows that are stored on the clipboard into the current targets. The point of insertion will be the currently selected row.

Insert Rows...

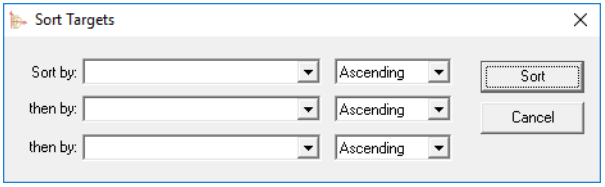
This command inserts a given number of rows above the current insertion point. The rows are interpolated so that the values in the Wavelength/Frequency column form an arithmetic or linear progression. Other attributes of the targets are also linearly interpolated.

Delete Rows...

This command deletes the selected rows. Note that clicking the selection box at the extreme left and using **<Del>** deletes a line.

Sort

Sort places the targets in order. When the Sort command is selected, you are asked to specify the sort order with the following window:

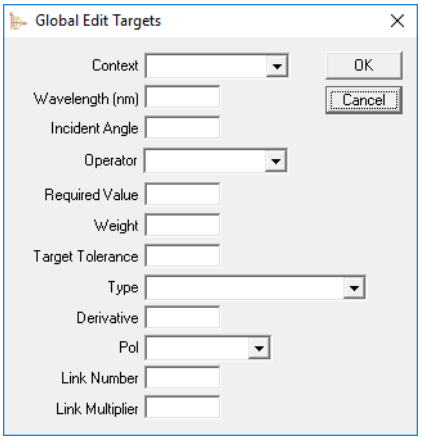


Targets may be sorted by the contents of up to three columns in either ascending or descending order. Once the columns have been selected, click **OK** to sort the targets. This command is particularly useful in conjunction with the Global Edit command where it used to group together the targets that are to be globally edited so that they may easy be selected prior to starting the global edit.

The Sort command applies to the current target window. For example, if the standard targets are displayed, then sorting will only apply to the standard targets.

Global Edit...

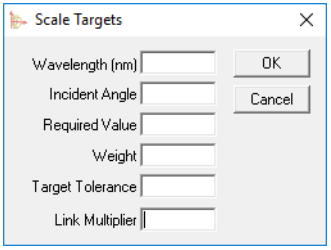
This command changes either all targets or selected targets only (if at least one target has been selected), to values entered on the Global Edit form.



If a value is entered into one of the fields, then the targets will be updated with the new value. If the field is left blank, then the value held in the targets will be not altered. Click OK to make the changes. Clicking Cancel causes the edit operation to be aborted.

Scale Targets...

This command is similar to the Global Edit command except that it multiplies the value in the target field by the value in the corresponding field of the Scale Targets form. The command changes either all targets or selected targets only (if at least one target has been selected).



For example, if 0.01 is entered into the **Required Value** field, then when **OK** is selected, the Required Value of the targets that are to be modified will be multiplied by 0.01.

Generate...

Generate helps in the setting up of a set of targets. The dialog box permits a range of wavelengths and/or a range of incident angles to be set with a particular performance specification. **Add** or **New** buttons are provided so that the results can just be added to the existing set of targets or can replace them.

The basic mode of operation is that each wavelength is given the range of angles specified. Be careful! This can generate a very large array of targets. For example, a range of wavelengths from 400 to 700 at steps of 20 together with a range of angles of incidence from 0 to 45 at intervals of 5 will give 160 separate targets. An alternative to specifying the step size is to specify the number of targets over the range by entering a number in the #points box.

To set a range of angles at one wavelength set the starting and ending wavelengths to the same value and similarly with specifications at just one angle.

The target generator can also create pairs of linked targets. To change to this mode, click **Linked Targets** (To change back to the basic mode, click **Regular Targets**). In this mode, there are two types of target: Primary and Secondary. The Primary target is the same as would be generated in the basic mode but with the addition of a **Link Multiplier**. The Secondary target is specified as an offset from the primary target in wavelength and incident angle. The two targets are linked together during target generation.

Display Wavelength

This command causes the targets to be displayed in terms of the wavelength parameter as defined in **General Units** on the **Options** menu.

Display Frequency

This command causes the targets to be displayed in terms of the frequency parameter as defined in the **General Units** on the **Options** menu.

Remove Duplicates

This command causes duplicate targets to be deleted. The default action is for duplicate targets to be automatically deleted, but in some cases it is preferable not to delete the duplicate targets as soon as they are detected (for example if you are pasting in a common range of values but want to change the polarization). **The Remove Duplicates Immediately** option in the **Targets** tab of the **General** options controls the automatic removal of targets. If this option is unchecked, then duplicate targets will not be automatically deleted. If duplicate targets are present when refinement is selected, a warning message will be displayed and refinement will be stopped.

Refinement and Synthesis

The eight classes of technique provided for refinement and/or synthesis are Simplex, Optimac, Simulated Annealing, Conjugate Gradient, Quasi-Newton, Needle Synthesis, Differential Evolution. and Non-Local Refinement. Simplex provides straightforward refinement, Optimac refinement and/or synthesis, Simulated Annealing refinement but over a wide region of parameter space, Conjugate Gradient and Quasi-Newton are refinement methods that use derivative information when determining how to modify the design. Needle synthesis is a method of adding layers to a design based upon the

derivative of the merit figure for a zero thickness layer. Differential Evolution attempts to evolve a population of designs towards a better solution. It also has the ability to search for designs that are less sensitive to independent errors. Differential Evolution potentially evaluates a substantially larger number of designs than the other techniques, and so can take much more time to find a solution. Non-Local Refinement repeated creates a random design (subject to specified constraints) and runs a specified refinement method on the randomized design. The best designs are kept in a history list for later examination.

The techniques can be selected from the Design Window **Tools** or **Parameters** menu. Selection through **Tools** activates the process directly. Selection through **Parameters** permits adjustment of the parameters of the appropriate process.

We first consider the various parameters that must be set and to help in understanding them we include a brief description of each technique.

Refinement Parameters

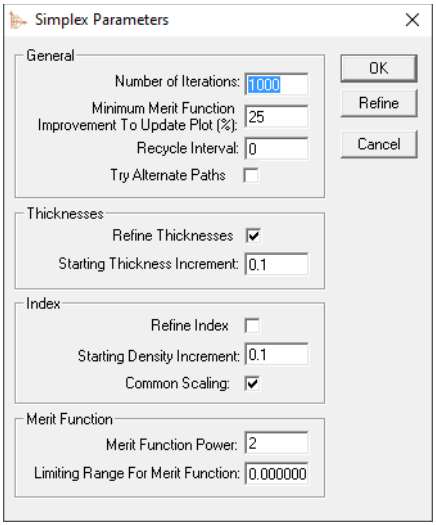
Simplex

Simplex refinement is very fast. A family of designs, the simplex, is set up by perturbing the layers and/or the packing densities of the starting design. Usually the total number of designs will be one more than the number of layers and packing densities with a minimum of five for very small numbers of layers. The refinement technique then consists of a process of exchanging the poorest design for a better one at each iteration. The better design is generated by reflecting the worst one in the center of gravity of the simplex, or, if that is not successful, by moving towards the center of gravity.

Simplex Parameters

Simplex parameters are set in a parameters dialog box (see next page).

Either or both **Refine Thicknesses** and **Refine Index** may be selected. In order that dispersive materials may be accommodated, the model used for the variation of refractive index is that of variable packing density. The model is detailed in the subsection **Packing Density** in the **Essential Macleod Structure** earlier in the manual. The starting thickness increment is the amount by which each layer is perturbed to set up the original simplex of designs. The packing density increment is likewise shown but there is an additional check box, **Common Scaling**. If this box is checked then the packing densities of all layers of the same material move together. This is useful in reverse engineering where deposition conditions may have caused all the layers of a particular material to vary in the same way from ideal. In reverse engineering the packing density range will be quite restricted. In index refinement the range can be made large. Inhomogeneity can be simulated by splitting each possibly affected layer into at least two parts each with its own packing density. The number of iterations determines the absolute limit to the refinement process. It should be set fairly large.



Simplex is very fast and each iteration is quickly over so a large number, several thousand, is recommended. It is always possible for the user to terminate the process earlier. For more complicated designs, the convergence can often be improved by recycling the simplex during refinement. The **Recycle Interval** parameter specifies the number of iterations between each automatic recycle. If this parameter is set to zero, then automatic recycling does not happen. **Try Alternate Paths** is used to make Simplex take into account the effect of a path selection on the next iteration. Sometimes the next iteration will achieve a better result if the best path is not taken in the current iteration. **Try Alternate Paths** allows Simplex to not take the current iteration's best path in this case.

Progress of the refinement is automatically displayed as a plot of performance. The plots will be produced each time the performance is improved by the amount in **Minimum Merit Function Improvement To Update Plot** since the last plot.

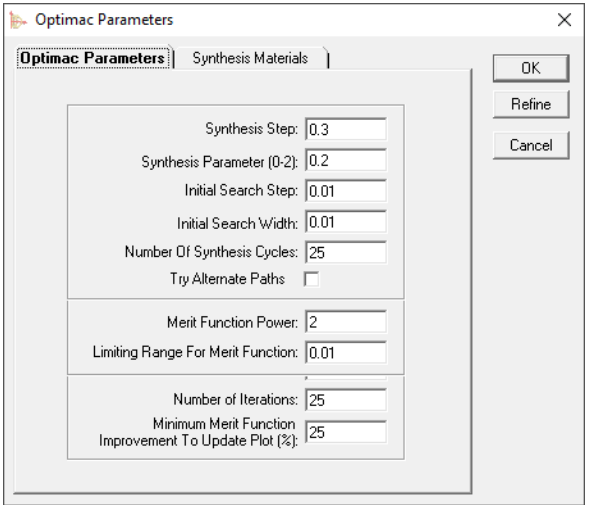
Use Custom Merit Function, **Source File**, and **Browse…** only apply to Designs and are only available when the Function enhancement is licensed. Information on the use of custom merit functions is included in the Scripting Language manual that is installed on your computer.

Optimac

Optimac has many facets. It possesses some aspects of a direction set technique but with a large number of different ways of constructing the conjugate search sets which are constantly changing in response to the progress of the refinement. As soon as one construction technique appears to be giving diminishing returns, another takes over. The method is appropriate for both synthesis and refinement. In synthesis there are rules for altering the design at the end of each refinement cycle by splitting layers, inserting layers, adding layers and even periodic random perturbation. The changes, however, are only provisional until proved to be useful by the subsequent progress of the process. If the promised improvements are not maintained then the current changes are dropped and a

different way of introducing the changes adopted. The process, therefore, is constantly altering itself in response to progress.

Optimac Parameters



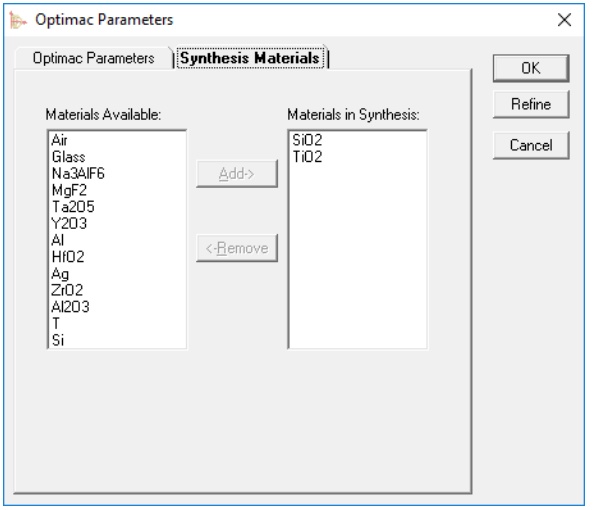
Optimac has no limits on layer thickness, except that they may not become negative, although thicker layers are more likely to be subdivided in the course of the synthesis. The parameters editor determines whether or not refinement or synthesis is involved by the value set for **Number of Synthesis Cycles**. *If this is zero then only refinement will be performed*. If synthesis is to be carried out then the value to insert depends very much on whether or not there is a good starting design. With virtually no starting design then a value of 50 or so is reasonable. With a good starting design, a lower figure can be used. The **Synthesis Step** represents the thickness of layers that are inserted in the synthesis process. This should normally be set quite large and 0.1 to 0.3 are good values. The **Synthesis Parameter** determines whether the changes will be retained in the synthesis operation. When a design is changed by adding or perturbing layers, the merit figure usually rises. A short process of adjustment then begins and continues as long as the improvement in the merit function continues to be satisfactory as defined by certain conditions on the relative improvement. If the resulting figure of merit is poorer than the old nevertheless the new design will be accepted provided the fractional increase in the figure of merit is not greater than the synthesis parameter. A value of around 0.2 or so is quite a good starting value. The **Initial Search Step** is the search interval for the first quick scan of the search direction. The initial search takes place over a width that is given by the current value ± the **Initial Search Width**. If convergence is good, this value can be set equal to the initial search step. If convergence is slow and performance improves only slowly then the search region can be greatly extended. During refinement, however, the interval is constantly adjusted on the basis of progress. **Try Alternate Paths** is used to make Optimac take into account the effect of a layer insertion method on the next iteration. Sometimes the next iteration will achieve a better result if the best layer

insertion method is not taken in the current iteration. **Try Alternate Paths** allows Optimac to not take the current iteration's best insertion method in this case.

The **Number of Iterations** refers to the refinement between each synthesis operation. This should be set to 40 or 50. The **Maximum Number of Layers** should not be set too large if the process is to be completely automatic, otherwise there may be a tendency to continue to add thin layers. If the process is to be monitored and stopped manually at an appropriate point then this can be large. Progress of the refinement is automatically displayed as a plot of performance. The plots will be produced each time the performance is improved by the amount in **Minimum Merit Function Improvement To Update Plot** since the last plot.

Use Custom Merit Function, **Source File**, and **Browse…** only apply to Designs and are only available when the Function enhancement is licensed. Information on the use of custom merit functions is included in the Scripting Language manual that is installed on your computer.

Click on the Synthesis Materials tab to control the materials that will be used by Optimac when inserting new layers.



Initially, all the materials in the design will be used for synthesis. Some of these materials may be removed or others not in the starting design may be added to the list. Clicking **OK** will save the parameters for future use. Clicking **Refine** will start synthesis.

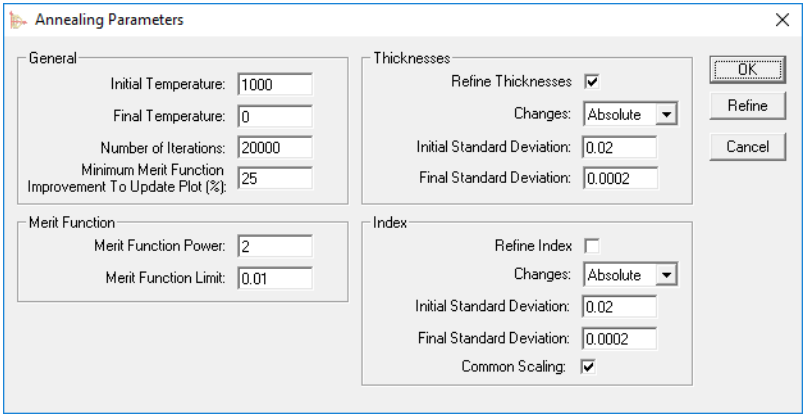
Simulated Annealing

Simulated Annealing is not a particularly new technique but it has not been much applied to thin film coatings. It consists of a design that is randomly perturbed to wander over the merit function surface. At each fresh perturbation, a new figure of merit is computed. Better designs are always accepted but poorer designs are sometimes accepted with a probability that is gradually reduced as the process continues. It attempts to mimic a real annealing process and the probability of accepting a poorer result is determined by

a random number drawn from a Boltzmann distribution, exp(-E/kT) where E represents the random increase in the merit figure and kT represents an "annealing temperature." (The k here represents the Boltzmann constant and *not* the extinction coefficient). The design gradually relaxes towards a minimum figure of merit. The longer the process is permitted to take usually the better the eventual minimum. Simulated annealing is at its best when there is no obvious starting design. It responds well to specifications that involve angle of incidence effects, especially ones where the other techniques are sluggish.

Annealing Parameters

The parameters that are to be specified are shown in the reproduction of the dialog box below.



The parameters, standard deviation and initial temperature, are specified separately. The standard deviation for the layer thickness fluctuations has a starting and a finishing value. Near the start of the operation the fluctuations should be fairly large but at the end large fluctuations tend to be nonproductive because they move the design to an extent that is unacceptable. It can be arranged, therefore, that the ending value is different from the starting. Similarly, the index variation has its own standard deviation, so that the index variations do not have to follow the same profile as the thickness variations. The annealing temperature is measured in degrees, each degree being 1/10000 of the starting figure of merit. Good starting values are in the hundreds or even thousands. The annealing process will gradually reduce the temperature to the end value which can conveniently be zero. The fall in temperature is not linear. The rate of decrease is somewhat greater at the start of the process than at the end, and it is the same with the standard deviation.

Absolute or relative changes determines how the random variations will be applied. For absolute changes in thickness the fluctuations are treated as absolute layer thickness changes, that is a fluctuation of 0.2 is treated as 0.2 x λ_0 added to the current thickness of the layer. If the changes are relative, it means that the layer thickness will be increased by 0.2 of its current value. Absolute is a better choice, at least for starting, otherwise thin layers will scarcely move. For absolute changes in packing density, the fluctuation is

added to the current packing density value, a fluctuation of 0.2 is treated as adding 0.2 to current value of packing density. For relative changes the packing density will be increased by 0.2 of its value.

In simulated annealing, the random walk process can very quickly move layers out against their constraints even when they are set very large. This creates problems. The technique used here, therefore, ensures that the layers are reflected in the constraints rather than simply being restrained by them. Because of this reflection the constraints can and should be set at a reasonable value. If they are set too large then, particularly at the early stages, the corresponding thick layers lead to tightly spaced fringes and sometimes quite wild oscillations of the figure of merit.

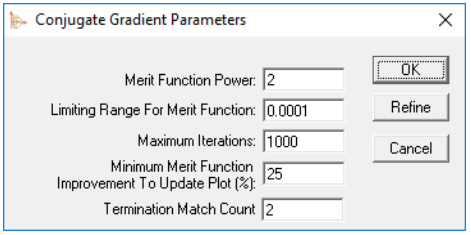
Progress of the refinement is automatically displayed as a plot of performance. The plots will be produced each time the performance is improved by the amount in **Minimum Merit Function Improvement To Update Plot** since the last plot.

Use Custom Merit Function, **Source File**, and **Browse…** only apply to Designs and are only available when the Function enhancement is licensed. Information on the use of custom merit functions is included in the Scripting Language manual that is installed on your computer.

Conjugate Gradient

The Conjugate Gradient refinement method belongs to the class of methods that use derivative information to determine the local slope of the Merit Function surface. This information is then used to change the design parameters (typically layer thicknesses) in an attempt to improve the design.

Conjugate Gradient Parameters



For Conjugate Gradient, the **Merit Function Power** must be a positive even number. The larger this is made, the more refinement works on the parts of the design that are furthest from the targets. In general, a value of 2 works well. **Limiting Range for Merit Function** is one of the termination criteria for Conjugate Gradient refinement. If the merit figure falls below this value, then Conjugate Refinement will terminate and return the refined design. **Maximum Iterations** is another termination criterion. If Conjugate Gradient refinement has made **Maximum Iterations** attempts to improve the design, then it will stop and return the refined design. **The Minimum Merit Function Improvement To Update Plot (%)** controls how often the progress plot is updated. Plotting can take a significant amount of time and if the merit figure has not significantly changed, then the plot will be very similar to the previous plot. To avoid unnecessary plots, a plot will not

be generated until the merit figure has decreased by the specified percentage amount from the merit figure value at the previous plot. The Conjugate Gradient progress window includes a **Plot Now** button so that you can look at changes before the necessary improvement has been made. Conjugate Gradient refinement also includes termination criteria based on the merit figure slope. If the slope value becomes small, the refinement will terminate because it assumes that it has found the best design. For some designs, however, this termination is too early. There can be long periods where the slope is very small, but after a while, the refinement finds a much larger slope that it then descends. For this reason, the **Termination Match Count** can be used to specify the number of consecutive times that the small slope requirement must be met before refinement terminates. If the **Termination Match Count** is set to less than zero, then refinement will never terminate because of a small merit figure slope.

Quasi-Newton

Quasi-Newton refinement also belongs to the class of methods that use derivative information to determine the local slope of the Merit Function surface. This information is used to change the design parameters (typically layer thicknesses) in an attempt to improve the design.

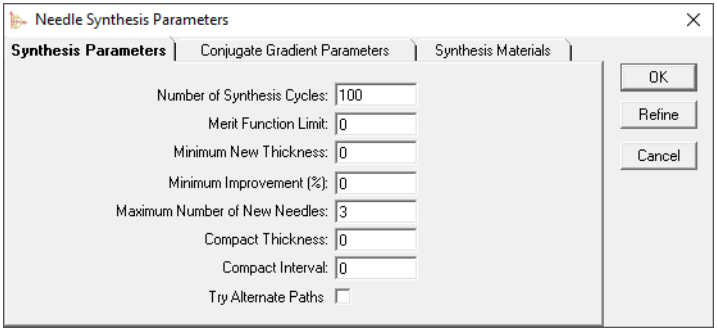
Quasi-Newton Parameters

The parameters for Quasi-Newton refinement are similar to the Conjugate Gradient refinement parameters. The exception is an extra parameter **Recycle Interval**. The convergence rate of Quasi-Newton can often be improved by restarting the refinement. The recycle interval parameter restarts the refinement every **Recycle Interval** iterations. The base value for this parameter is difficult to determine, but a value between 15 and 20 often works well. Setting the value to 0 stops automatic recycling.

Needle Synthesis

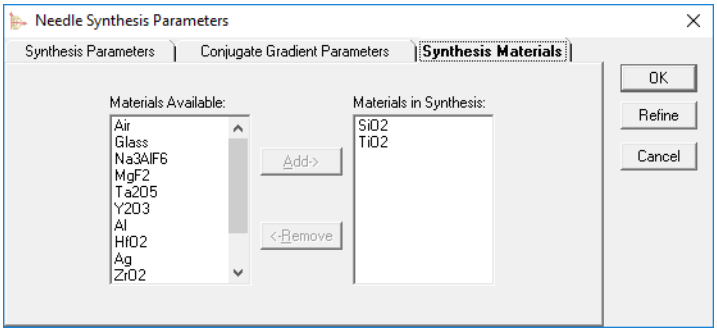
Needle synthesis uses derivative information from the merit figure surface to determine where to insert new layers. The derivative of the merit figure with respect to layer thickness for a zero thickness layer is calculated as the zero thickness layer is moved through the existing layers. The best places to insert new layers are given when the merit figure derivative is most negative. More than one zero-thickness layer can be inserted at a time. After all zero-thickness layers have been inserted, Conjugate Gradient refinement is used to expand the thicknesses of the new layers to non-zero values. During refinement, other layer thicknesses may also change thickness if it improves the merit figure. The process is repeated until the desired design is achieved or the process reaches some limit such as total number of iterations.

Needle Synthesis Parameters



The **Number of Synthesis Cycles** parameter specifies the number of times that Needle Synthesis will attempt insert layers. When this parameter has been exceeded, Needle Synthesis will stop. The **Merit Function Limit** is another parameter that controls when Needle Synthesis stops. When the merit figure falls below this value, Needle Synthesis will stop. If after Conjugate Refinement has completed, the newly inserted layers have a thickness less than the **New Thickness Value**, then Needle Synthesis will add extra material to either the layer next to the incident medium or the layer next to the substrate. This gives Needle Synthesis extra material to search when looking for a place to add a new layer. If the merit figure has not improved by the amount specified by **Minimum Improvement**, then again, extra material will be added to the design to provide more search space. **Maximum Number of New Needles** specifies the maximum of new layers that will be added at each iteration. When **Compact Interval** is greater than zero, every **Compact Interval** iterations, Needle Synthesis will compact the design, removing layers whose thicknesses are less than **Compact Thickness**. If **Compact Interval** is zero, then the design is never compacted. **Minimum New Thickness** and **Compact Thickness** are always in units of nanometres. **Try Alternate Paths** is used to make Needle Synthesis take into account the effect of needle insertions on the next iteration. Sometimes the next iteration will achieve a better result if the best set of needles is not taken in the current iteration. **Try Alternate Paths** allows Needle Synthesis to not take the current iteration's best needle set in this case.

The Conjugate Gradient Parameters tab contains the same parameters as described for Conjugate Gradient above in this manual.



The Synthesis Materials tab lists the materials that are to be used when inserting layers into the design. By default, the materials to be used are all the layer materials in the design that are not in locked layers. You can add or remove materials from the list, by selecting each material and then clicking **Add** or **Remove**.

Differential Evolution

Differential Evolution is an evolutionary optimization algorithm. It attempts to find better solutions to a problem by modifying a population of designs through mutation and selection of the best designs. The process begins by creating a population of designs with random thicknesses and/or packing densities and/or materials based on the starting design. The limits on thicknesses and densities are specified either by the maximum and minimum limits in the design or by the error parameters. Materials are chosen from a specified list of materials.

The process then repeatedly creates a new generation of designs from the previous generation until either the maximum number of generations has been created or a design with a sufficiently small merit figure has been found. The process will also end if the difference between the merit figures of the best and worst designs in the current generation falls below a user-specified value. This allows the process to stop if it has converged on a single design, but that design does not meet the sufficiently small merit figure requirement.

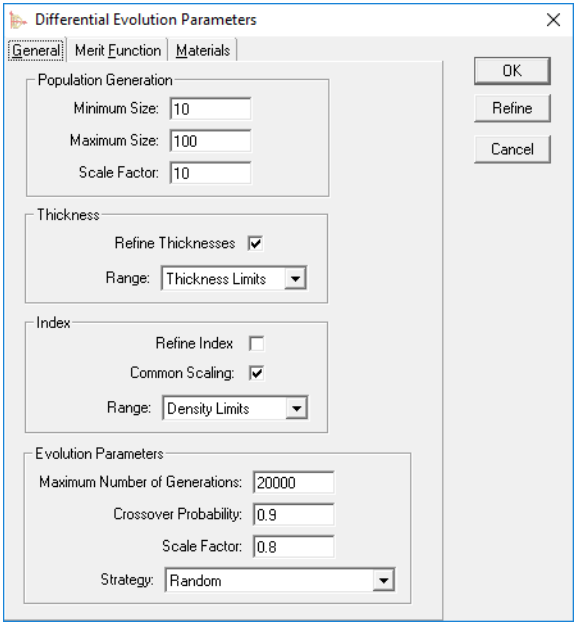
In the standard method the next generation is formed by considering each design in the population in turn. A new design is created from the previous generation by randomly selecting three designs. The first of these designs is modified by taking each parameter in turn. A Crossover probability determines if the parameter will be modified or not. If the parameter is to be modified then the modification is performed by taking the difference of the same parameter in the second and third designs, multiplying that difference by a scale factor and then adding the result to the parameter in the first design. The complete mutated first design is then compared with the design under consideration. If the mutated first design has a lower merit figure than the design under consideration, then the design under consideration is replaced by the mutated design, otherwise the design under consideration is kept in the new generation. The new generation is complete when all designs in the population have been considered,

If any of the stopping criteria have been met, the process ends, otherwise it will start creating the next generation.

The Differential Evolution technique also supports searching for designs that are less sensitive to independent errors. Normally a merit figure is calculated for a single design and that figure represents how well the design matches the targets. When searching for designs that are less sensitive to errors, the single design is perturbed several times in the same way that the independent errors tool perturbs a design. The merit figures of each of these perturbed designs are calculated. The worst merit figure calculated is the merit figure of the single design. This sensitivity reduction feature is not available in vStack.

Differential Evolution potentially evaluates a substantially larger number of designs than the other techniques and so can take much more time to arrive at a solution.

Differential Evolution Parameters



The **Population Generation** section controls the size of the design population. The size of the population is constrained to be at least **Minimum Size** members and no greater than **Maximum Size** members. Subject to these constraints, the population size is calculated from **Scale Factor** x number-of-parameters where number-of-parameters is the sum of the number of different thicknesses to be refined and the number of different densities to be refined. A **Scale Factor** of 10 is a useful starting point.

The **Thickness** section controls refinement of thicknesses. Check **Refine Thicknesses** to allow thicknesses to take part in the refinement. **Range** controls the limits from which the initial random population is drawn. When **Range** is set to **Thickness Limits**, the thickness limits are given by the Minimum and Maximum Physical or Optical Thickness Limits in the Design window. When **Range** is set to **2 x Error Limits**, the thickness limits are given by the parameters in the Errors tool. The minimum thickness will be given by the thickness 2 standard deviations below the mean error and the maximum thickness will be given by the thickness 2 standard deviations

above the mean error. When **Range** is set to **3 x Error Limits**, the minimum thickness will be given by the thickness 3 standard deviations below the mean error and the maximum thickness will be given by the thickness 3 standard deviations above the mean error.

The **Index** section controls refinement of packing density. Check **Refine Index** to allow packing densities to take part in the refinement. **Range** controls the limits from which the initial random population is drawn. When **Range** is set to **Density Limits**, the density limits are given by the Minimum and Maximum Density Limits in the Design window. When **Range** is set to **2 x Error Limits**, the density limits are given by the parameters in the Errors tool. The minimum density will be given by the density 2 standard deviations below the mean error and the maximum density will be given by the density 2 standard deviations above the mean error. When **Range** is set to **3 x Error Limits**, the minimum density will be given by the density 3 standard deviations below the mean error and the maximum density will be given by the density 3 standard deviations above the mean error. When **Common Scaling** is checked, layers of the same material will always have the same packing density.

The **Evolution Parameters** section controls the strategy used. When **Maximum Number of Generations** has been reached, the refinement will stop. **Crossover Probability** controls the proportion of parameters in each design that will be modified. 0.9 is a good starting point. **Scale Factor** controls the random variability of designs. A larger **Scale Factor** generates design populations with more variability. Generally the **Scale Factor** should be value a between 0 and 1 but it can be larger than 1. 0.8 is a good starting point. When the **Strategy** is **Random per Generation Dither**, 0.3 is a good starting point. The **Strategy** controls the method used to generate new designs. The **Random** strategy is the method described above and is probably the best to try first.. **Local to Best** is a modification that attempts to balance robustness in finding the best solution with fast convergence. **Best** is designed for small population sizes and fast convergence. The number of layers to be refined should not be too large. **Random per Vector Dither** uses the same strategy as **Random**, but the **Scale Factor** has a small jitter applied to it. The **Scale Factor** is randomly altered each time a design is generated. In **Random per Generation Dither** the **Scale Factor** is randomly altered at the beginning of each generation. **Random Either Or** randomly alternates between using the difference of two parameters as in the **Random** strategy and using three parameters.

The **Merit Function** tab controls the properties of the Merit Function. The refinement will stop when the merit figure reaches a value of **End When Merit Figure <** or less. The refinement will also stop when the difference between the best and worst merit figures in the current generation is less than **End When Merit Figure Range <**. This value is normally very small so that refinement will stop when all the population members have the same parameter values, that is, they all represent the same design.

Progress of the refinement is automatically displayed as a plot of performance. The plots will be produced each time the performance is improved by the amount in **Minimum Merit Function Improvement To Update Plot** since the last plot.

When **Number of Trials** is 0, Differential Evolution will calculate a merit figure based solely on the trial design as is performed with the other refinement methods. When **Number of Trials** is greater than zero, **Number of Trials** perturbed designs will be created from the trial design. The merit figures of each of these designs will be calculated

and the worst merit figure will be assigned to be the merit figure of the trial design. This causes the refinement to prefer designs that are less sensitive to errors. The perturbed designs are created in the same way as the Errors tool and use the parameters in the Errors tool dialog to control the perturbations. **Re-randomize** controls the generation of the random numbers used to create the perturbed designs. When set to **Never**, the set of random numbers is generated once and used for the whole refinement. In this case, the same design will have the same merit figure throughout the refinement. When set to **Each Generation**, a new set of random numbers is generated at the beginning of each generation. In this case the same design will have the merit figure within a generation, but could have different merit figures in different generations. When set to **Each Mutation**, a new set of random numbers is created each time a design is mutated. In this case, the same design could have different merit figures within the same generation. These parameters cannot be set in Differential Evolution for vStack.

Use Custom Merit Function, **Source File**, and **Browse…** only apply to Designs and are only available when the Function enhancement is licensed. Information on the use of custom merit functions is included in the Scripting Language manual that is installed on your computer.

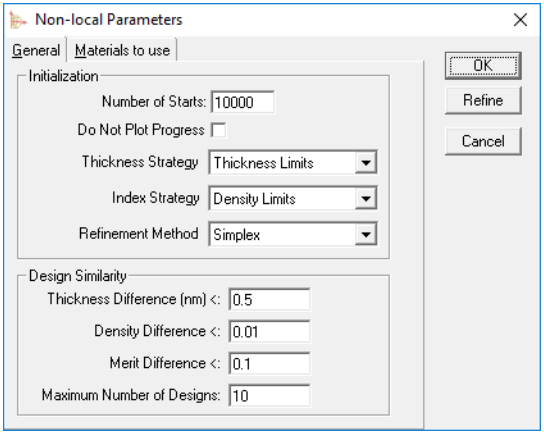
The **Materials** tab specifies if Differential Evolution is permitted to alter the layer materials during optimization and if so, which materials can be used for each layer. When **Change Materials in Layers** is checked, the materials used for each layer can be changed during optimization. The **Materials to Use** list specifies the materials that can appear in the design.

Non-Local Refinement

The refinement techniques above except for Differential Evolution and Optimac move the design to a nearest minimum. The path to the minimum is potentially different for each technique and so it is possible for each technique to finish at a different minimum. In general, there are many minima for a design and so where a design is far from a potential good minimum it is possible that refinement might not finish in the best minimum. That is, the refinement is sensitive to the starting point of the design.

Ways of improving the chance of finding the best minimum include using statistics-based techniques such as Simulated Annealing and Differential Evolution. Another way is to use the other refinement methods with many different starting points. Non-local refinement implements this method.

Non-Local Refinement Parameters



The parameters for non-local refinement are divided into three parts: specifying the starting points with refinement technique to be used, specifying the criteria that determine if two designs are the same, and specifying if materials can be changed and which materials to use.. **Number of Starts** defines the number of starting designs that will be created. **Thickness Strategy** controls the limits of the random thickness generation. When **Thickness Strategy** is set to **Thickness Limits**, the thickness limits are given by the Minimum and Maximum Physical or Optical Thickness Limits in the Design window. When **Thickness Strategy** is set to **2 x Error Limits**, the thickness limits are given by the parameters in the Errors tool. The minimum thickness will be given by the thickness 2 standard deviations below the mean error and the maximum thickness will be given by the thickness 2 standard deviations above the mean error. When **Thickness Strategy** is set to **3 x Error Limits**, the minimum thickness will be given by the thickness 3 standard deviations below the mean error and the maximum thickness will be given by the thickness 3 standard deviations above the mean error.

Index Strategy controls the limits of the random packing density generation. When **Index Strategy** is set to **Density Limits**, the density limits are given by the Minimum and Maximum Density Limits in the Design window. When **Index Strategy** is set to **2 x Error Limits**, the density limits are given by the parameters in the Errors tool. The minimum density will be given by the density 2 standard deviations below the mean error and the maximum density will be given by the density 2 standard deviations above the mean error. When **Index Strategy** is set to **3 x Error Limits**, the minimum density will be given by the density 3 standard deviations below the mean error and the maximum density will be given by the density 3 standard deviations above the mean error.

Plotting the progress of designs during refinement can consume a significant amount of time. Checking the **Do Not Plot Progress** option prevents design performance from being plotted and can significantly improve refinement times.

Whether or not the thickness values are refined and whether or not the packing density values are refined depends upon the capabilities of the selected **Refinement Method** and how the parameters for the particular method have been set. The methods available are:

Simplex, **Optimac**, **Conjugate Gradient** and **Quasi Newton**. When **Optimac** has been selected, the **Number of Synthesis Cycles** is always treated as zero regardless of the value set in the Optimac Refinement Parameters.

The termination criteria for each of the refinement methods will generally allow the refinement to end when the design is near the minimum. If refinement approaches the same minimum from different directions, it is likely that it will terminate at slightly different designs. Thus when comparing if two designs are equal, it is necessary to allow for some tolerances in different thicknesses, packing densities and merit figures. This is the purpose of the **Design Similarity** section. For each of the top three parameters a maximum difference is specified. If any of the layer thicknesses, layer packing densities or merit figures of a pair of designs exceed these differences then the designs are not considered to be identical.

The **Materials** tab specifies if non-local refinement is permitted to alter the layer materials during the creation of the starting point and if so, which materials can be used for each layer. When **Change Materials in Layers** is checked, the materials used for each layer can be changed when the starting design is being created. The **Materials to Use** list specifies the materials that can appear in the design.

A history of designs is maintained. The history list retains up to **Maximum Number of Designs** designs that are considered different according to the **Design Similarity** criteria. For each retained design, the history list shows the number of times refinement has finished at that design and the merit figure of the design. Double-clicking on the row in the history list will open the design for inspection and optional saving. The design history list cannot be saved. When the design history list is closed, all the designs in the list will be lost (except for those previously saved).

Refinement and/or synthesis progress

All displays give a graph of the best current performance. The scales for the graph are taken from the design's performance parameters. Where appropriate, the values of the targets are indicated on the graphs.

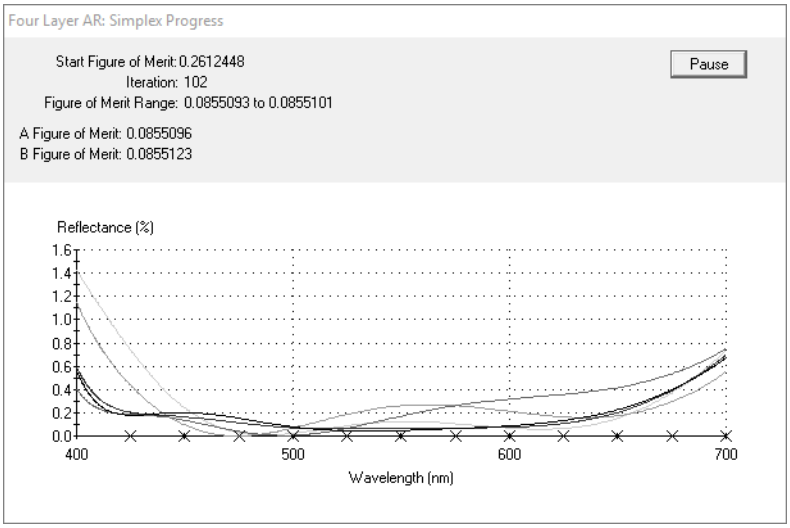
Above the graph there is a data window that presents details of the refinement progress and it is here that the various displays differ.

Once the refinement or synthesis is under way it will terminate without supervision when criteria set in the parameters editor are satisfied. These depend on the particular technique but they involve a target figure of merit, or a certain number of iterations or cycles, or a certain range of the figures of merit. However, some control can be exerted on it as it proceeds and this may be of benefit to the process. The control involves selecting the pause button that is at the top right of the display. This presents the user with a number of options that depend to some extent on the technique. All include the option to terminate the process either accepting the best design so far or returning to the starting design. It is also possible to recycle the process. This means simply resetting a number of the parameters so that the refinement is effectively restarted from the beginning but adopting as starting design the best current one. This works very well in Simplex where a periodic disturbance of this type helps to improve the convergence and is recommended. In some of the processes it is possible to change a number of the

parameters of the refinement. Finally it is possible to resume the process with no changes at all.

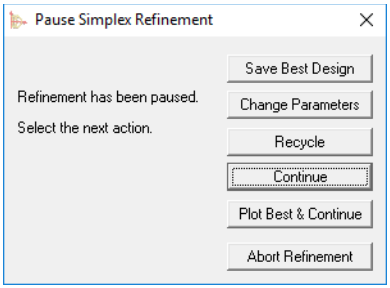
Simplex Progress

The display below shows the current range of figures of merit together with the results of the current assessment of a replacement design. The first choice is the design reflected in the center of gravity and this is indicated by the letter A. Should A be acceptable then a further assessment of a design that goes even further (twice as far) in the same direction is shown as B. The better of A or B is accepted. Should A be unsatisfactory then a design that is half way from the existing design to the center of gravity is assessed as design C. If this is better it will be accepted. Should neither A nor C be acceptable it is a sign that the extent of the simplex is greater than a simple merit function minimum and so the simplex should be reduced in size. All designs are then moved towards the best design and the process then continued.



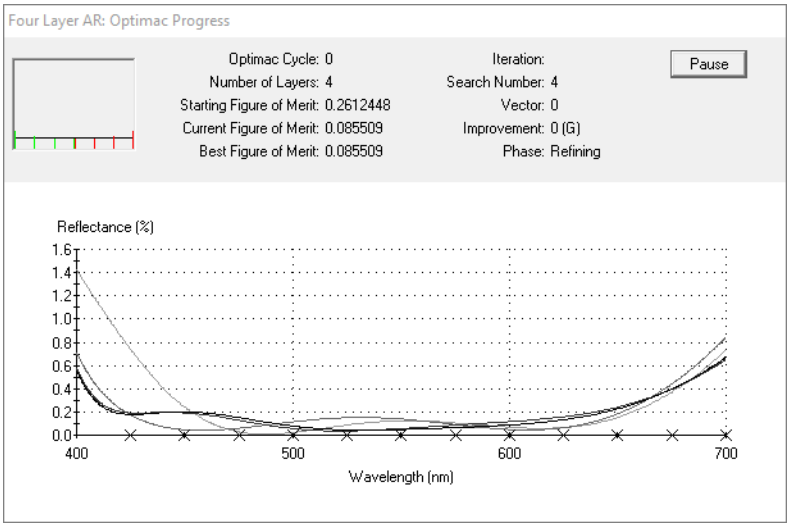
The plot of the performance of the current design uses the parameters that have already been set up for performance calculations.

The pause button at the upper left brings up a pause box with a number of options. The refinement may be terminated with either the preservation of the best design or a return to the starting design. The refinement parameters may be changed without terminating the process. The recycle command starts up a completely fresh simplex based on the current best design and helps to revitalize the convergence if it has become sluggish. In fact it is recommended that recycle should be activated at least once towards the end of the process.



Optimac Progress

Optimac shows a number of entries in a window displaying the performance curve. The particular entries depend on the stage of the process. A typical display might be as shown.



The upper line shows the cycle and iteration numbers. On the next line are the current number of layers and the search number. A cycle number indicates that this is synthesis. Optimac refinement is indicated by the term Optimac Progress instead of Optimac Cycle. Refinement rather than synthesis is selected by entering zero for the number of synthesis cycles in the parameters dialog box. The iteration number gives the number of iterations so far completed in the current synthesis cycle, that is in the refinement that follows a change in the number of layers.

At each iteration, a number of directions in parameter space equal to the number of layers is searched. These directions are set up in different ways and the search number indicates which direction is currently being searched. The progress of the search is indicated in the small display box at the top right of the progress window. This shows the various evaluations of the merit function as vertical lines that are either green or red

plotted against the magnitude of the current displacement vector. Green indicates a negative vector and red a positive. Note that this does not mean that the layers are necessarily thinner or thicker. The vector positive direction in parameter space is quite arbitrary. The dark line across the lower part of the progress box indicates the current best figure of merit and gives an idea of scale. The vector scale is simply arranged so that the width corresponds to the searched region. Sometimes it will be clear that the region actually searched is smaller and this indicates that over the missing part at least one of the thicknesses involved became negative.

Starting, current, and best figure of merit are self-explanatory. The vector shown corresponds to the best value for the particular search direction. The improvement displayed is unity if the current reduction in the figure of merit represents 1% of the limiting range for the merit function scaled to take account of the current merit function. For example, if the limiting range is 0.1 then RI of 1.0 indicates an improvement of 0.001, or 0.1%, in the current figure of merit. If the relative improvement falls below 1.0 then the current direction set is considered to be failing and, after an evaluation procedure, a different technique is substituted unless the procedure indicates that it is worth continuing with the current one. The particular procedure is indicated in parentheses after the improvement figure. G (standing for gradient) is the simplest and represents changes in just one single layer at a time. If the changes in the layers are small then G reproduces roughly the same alterations as does one of the gradient methods. C indicates that the directions within the set are being changed. The way in which they are changed ensures the generation of a conjugate set. A indicates no change in the set. B and BMod represent a number of alternative sets, BMod being not just one but several different sets and Rand represents a completely random but mutually orthogonal set. All of these are either changed, based on the current results when the letter C is displayed, or retained unchanged, when the letter A is displayed. The details of the sets are unimportant from the user's point of view but the technique can be thought of as constantly probing and searching in new directions to reach deeper and deeper levels of the merit function.

The synthesis is made up of a number of phases. These are indicated by **Phase**, just below **Improvement**. **Refinement** indicates a period of refinement with the number of layers remaining constant. At the end of each set of iterations that make up a synthesis cycle the **Inserting Layers** phase is entered. Here, layers that are not useful in maintaining the figure of merit are removed and others are added. The added layers at this stage have thicknesses corresponding to the synthesis step. A number of different techniques based on experience are used for adding the layers and several may be involved. Sometimes the design is also deliberately perturbed. Immediately after the additions the merit figure, and the number of layers, will usually show increases. The effect of the changes is then assessed in an operation known as **Initialization** that measures the rate of merit improvement and accepts the changed design only if the rate is considered satisfactory. Then the refinement portion of the cycle will recommence. Otherwise an alternative systematic phase known as a **Screening Search** will be initiated. This screening search begins by discarding useless layers and then explores a large number of alternatives but is triggered only when the normal processes of addition and perturbation fail.

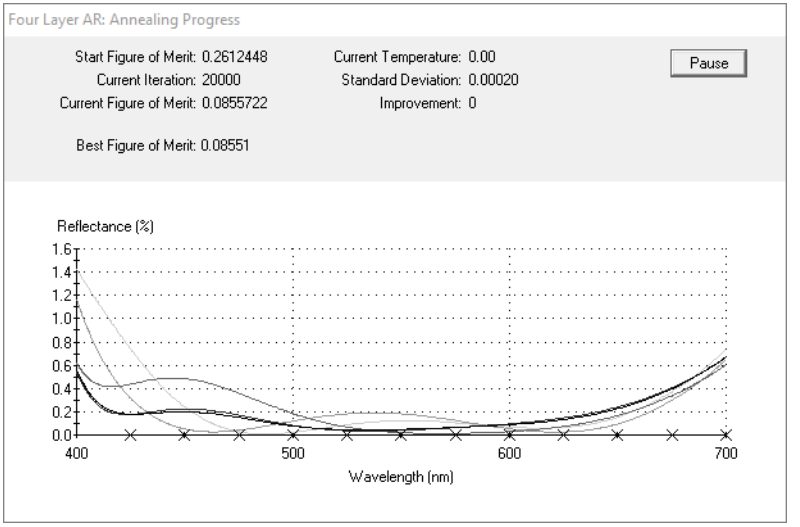
The process may terminate in several ways. If the merit figure falls below the set range or if the number of cycles exceeds the number entered then the termination will be

automatic. Often, however, the process may be terminated manually. This can be done by selecting the pause button which brings up a pause box similar to that for simplex.

When the process terminates it may be, if the synthesis parameter is large or if the termination occurs during an initialization, that an earlier cycle had a better figure of merit. If so this will be pointed out and the opportunity given to accept the better earlier design rather than the poorer later one.

Annealing Progress

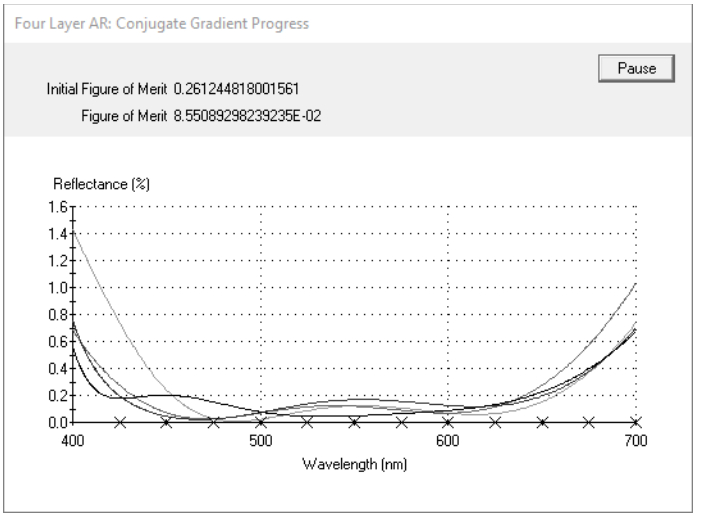
Simulated Annealing has a similar display, shown below, although the various entries are different in detail.



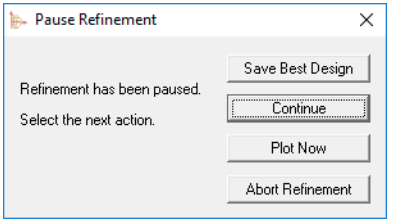
The current figure of merit is that calculated for the latest perturbation of the design. If this figure of merit is an improvement on the existing one then it will be accepted and the improvement item will show briefly a positive figure. If the figure of merit is worse than the current one then it may be accepted with a probability determined by the Boltzmann function. Then the improvement will show briefly a negative value. The best figure of merit indicates the lowest merit figure so far which is being held until a still better figure is achieved

Conjugate Gradient Progress

The Conjugate Gradient display is relatively simple. The figure of merit at the start of refinement is displayed together with the current figure of merit.



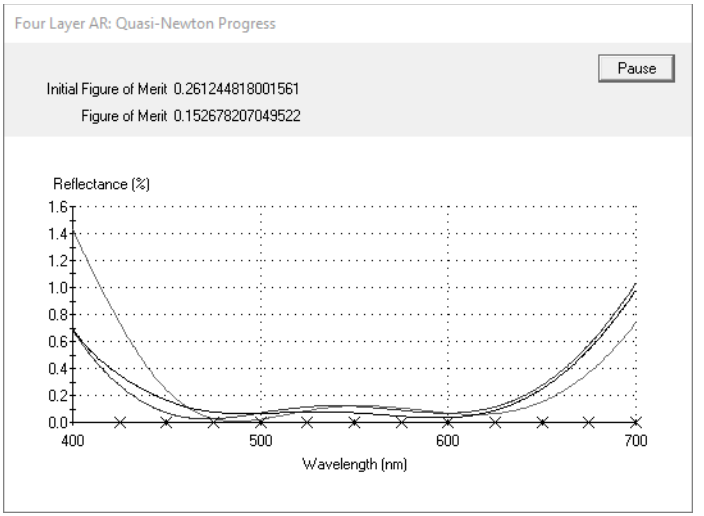
Clicking the Pause button displays the following options:



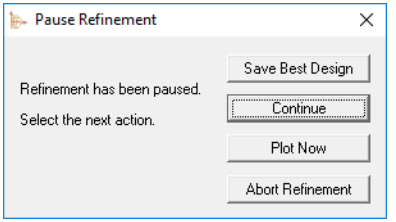
Selecting **Save Best Design** stops the refinement and stores the best design in the design editor. **Continue** closes the window and continues refinement. **Plot Now** causes the progress display plot to be updated with the performance of the current design. **Abort Refinement** stops refinement but does not change the contents of the design window.

Quasi-Newton Progress

The Quasi-Newton display is relatively simple. The figure of merit at the start of refinement is displayed together with the current figure of merit.



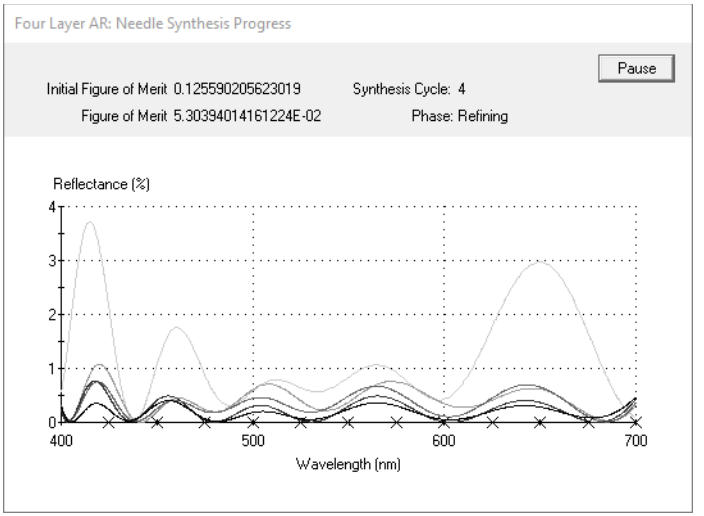
Clicking the Pause button displays the following options:



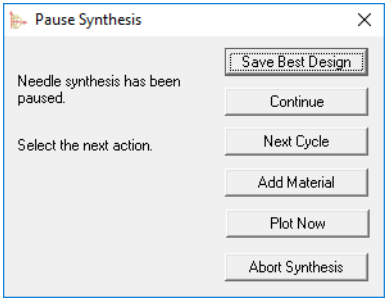
Selecting **Save Best Design** stops the refinement and stores the best design in the design editor. **Continue** closes the window and continues refinement. **Plot Now** causes the progress display plot to be updated with the performance of the current design. **Abort Refinement** stops refinement but does not change the contents of the design window.

Needle Synthesis Progress

The Needle Synthesis display is shown below. The figure of merit at the start of refinement is displayed together with the current figure of merit. The current synthesis cycle number is also displayed together with the current phase of synthesis. The displayed phases are *Adding Layers* shown when Needle Synthesis is determining where to add layers, *Refining* when Needle Synthesis is performing Conjugate Gradient refinement and *Compacting* when Needle Synthesis is removing thin layers.



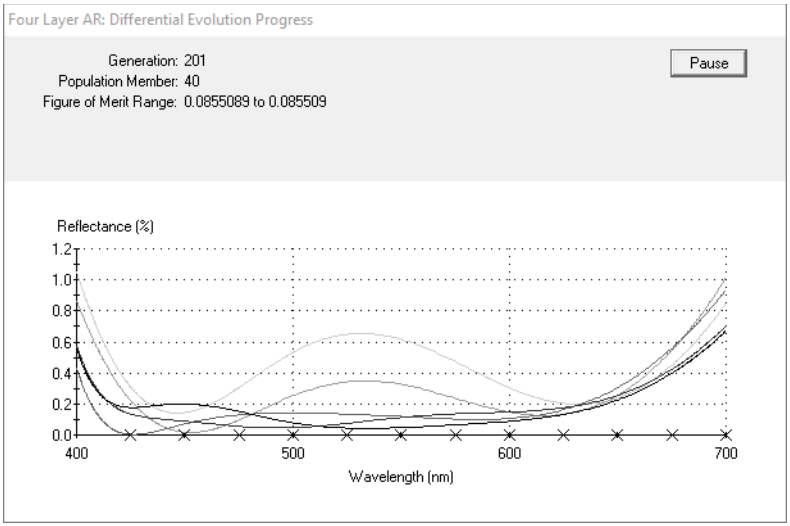
Clicking the Pause button displays the following options:



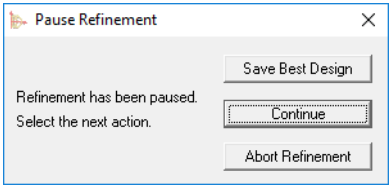
Selecting **Save Best Design** stops the synthesis and stores the best design in the design editor. **Continue** closes the window and continues synthesis. **Next Cycle** causes synthesis to begin the next synthesis cycle by adding new layers. **Add Material** forces Needle Synthesis to add extra material to one end of the design. **Plot Now** causes the progress display plot to be updated with the performance of the current design. **Abort Synthesis** stops synthesis but does not change the contents of the design window.

Differential Evolution Progress

The Differential Evolution display is shown below. The current generation is displayed together with the current population member being evaluated. Finally the current best and worst merit figures in the current generation are also shown.



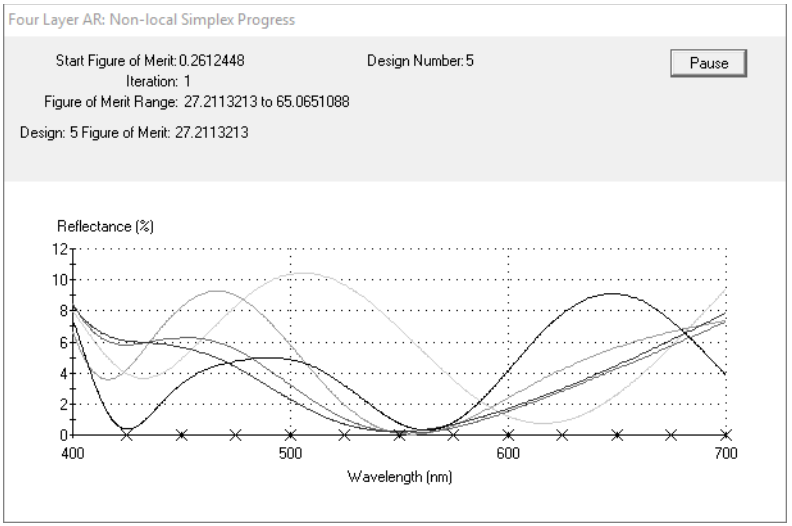
Clicking the Pause button displays the following options:



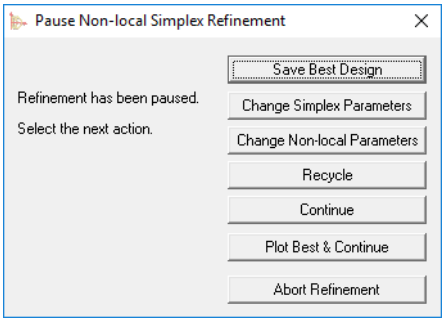
Selecting **Save Best Design** stops the refinement and stores the best design in the design editor. **Continue** closes the window and continues refinement. **Abort Refinement** stops refinement but does not change the contents of the design window.

Non-Local Refinement Progress

The Non-Local Refinement display is shown below



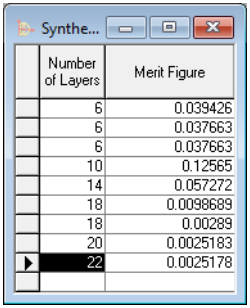
The display of data depends to some extent on the refinement method used. Simplex is shown. Because of the possible volume of calculation it is possible to suppress the plotting of the characteristic altogether. Then the display is as shown, but with a blank plot area. The Pause button activates the following dialog. Save Best Design saves the current best design and continues refinement with a subsequent design. Abort Refinement saves the current design and stops the process.



Archival Synthesis

A problem with virtually all synthesis techniques, not only in the thin-film coating field, is to decide when the process should be stopped. A more complex design gives improved performance, but there comes a point where the increase in complexity may be no longer worth the corresponding gain in performance. The recognition of this point is very much a subjective process that is almost impossible to program automatically into an automatic procedure. An advantage that the synthesis methods in the Essential Macleod have over many other current techniques is that there is a steady progression of

optimized designs characterized by increasing levels of performance accompanied by the expected increase in complexity.



During synthesis, the complete record of all optimized designs is retained and presented in summary form in a table. The example shows the record of an antireflection coating with target performance of a reflectance of zero over the region 400 to 1200nm. Materials used are specified as MgF2 and ZrO2. The Synthesis History window shows the figure of merit against the number of layers. The figure of merit shows a continuous fall while the number of layers fluctuates. This behavior is quite normal. The most attractive design from the point of view of performance against complexity is probably that of 11 layers with figure of merit 0.52791. Simply by double-clicking in the appropriate cell, the design can be recalled.

Any or all of the designs can be recalled and saved in regular design files so that they are preserved, but once the Synthesis History window is closed, any archived designs that have not been recalled and saved will be lost.

MATERIALS MANAGEMENT

Like real thin film materials those used in the package are absorbing and dispersive.

The refractive index component of the optical constant data is held in one of several models: Sellmeier coefficients, Cauchy coefficients, Drude coefficients, Lorentz coefficients, Drude-Lorentz coefficients, Hartmann coefficients or tabular data. The extinction coefficient component is either held as a table or can be declared to be zero. For Drude, Lorentz, and Drude-Lorentz, the extinction coefficient component is part of the model and so there is no separate extinction coefficient model.

The Sellmeier model is defined as:

$$n(\lambda) = \sqrt{1 + \sum_q \frac{A_q \lambda^2}{\lambda^2 - B_q}}$$

Where n is the refractive index, λ is wavelength, A and B are the Sellmeier coefficients and B is always in units of μm^2.

The Cauchy model is defined as:

$$n(\lambda) = \sum_q \frac{A_q}{\lambda^{2q}} \quad q = 0,1,2, \ldots$$

Where n is the refractive index, λ is wavelength, A is the set of Cauchy coefficients and is always in units of μm^{2q}.

The Drude model is defined as:

$$n^2(\lambda) = A - \frac{\lambda^2}{B^2(1 - i\lambda C)}$$

Where n is the complex refractive index, λ is wavelength, A, B, C are the Drude coefficients. A is theoretically unity (but may be greater than unity for real materials). B is the plasma wavelength in nm and C represents frictional loss.

The Lorentz model is defined as:

$$n^2(\lambda) = A + \sum_i \frac{B_i C_i \lambda^2}{\lambda^2 - C_i^2(1 + i\lambda D_i)}$$

Where n is the complex refractive index, λ is wavelength, A, B_i, C_i, D_i are the Lorentz coefficients. A is theoretically unity (but may be greater than unity for real materials especially when high frequency oscillators are not included in the summation). B_i is a combination of the plasma wavelength and the contribution of the *i*th term to the refractive index. C_i is the resonant wavelength of the *i*th term and D is the frictional loss of the *i*th term.

The Drude-Lorentz model is defined as:

$$n^2(\lambda) = A - \frac{\lambda^2}{B^2(1 - i\lambda C)} + \sum_i \frac{B_i C_i \lambda^2}{\lambda^2 - C_i^2(1 + i\lambda D_i)}$$

Where the parameters have the same meanings as above.

The Hartmann model is defined as:

$$n(\lambda) = A + \frac{B}{\lambda - C}$$

Where n is the refractive index, λ is wavelength, A, B and C are the Hartmann coefficients and C is always in units of μm.

When the refractive index model is not Drude, Lorentz, or Drude-Lorentz, the extinction coefficient is either held as a table of values or a Cauchy model or an exponential model or declared to be zero.

The Cauchy model for extinction coefficient is defined as:

$$k(\lambda) = \sum_{q} \frac{A_q}{\lambda^{2q}} \quad q = 0,1,2, \ldots$$

Where k is the extinction coefficient, λ is wavelength, A is the set of Cauchy coefficients and is always in units of μm^{2q}.

The exponential model for extinction coefficient is defined as:

$$k(\lambda) = Ae^{\frac{B}{\lambda}}$$

Where k is the extinction coefficient and A and B are constants.

For isotropic materials, there is one set of data. For anisotropic materials there are three sets of data, one set for each principal axis. The same data model must be used for each axis.

In calculations, for the Sellmeier, Cauchy, Drude, Lorentz, Drude-Lorentz and Hartmann models, the refractive index is calculated from the coefficients. For the table model, the required values are read from the tables. If necessary the values are interpolated or extrapolated. Interpolation is linear. Extrapolation keeps the last value from the table. The wavelengths do not need to be equally spaced. Where the values of *n* and/or *k* are changing rapidly, for example, the density of values can be greater. Similarly for the Cauchy and exponential models the extinction coefficient is calculated from the coefficients.

Tables are provided as well as the dispersive formulae because of the wide range of different materials and conditions that are involved. Some metals, for example, cannot be represented by the common normal dispersion formulae that are useful only for very well behaved dielectric materials over limited spectral regions. Any material can be represented by a table.

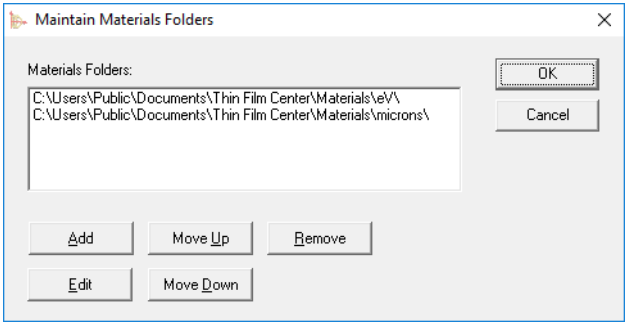
The tables of values need to be maintained. It must be possible to extract and examine the values that are stored. Changes may be necessary. New materials may have to be added. Unnecessary materials may have to be deleted. A new database of materials based on an existing one, perhaps a subset, may need to be constructed. All of these operations are included in the package.

The Materials Database

Each materials database consists of a collection of material files, with an index, in a separate folder. The number of databases is limited only by the capacity of the hard drive. Only one materials database can be active at any one time but a need for a design to use materials from several databases can be very easily accommodated by importing the relevant materials files, a simple and rapid operation.

The active database is set in the Essential Macleod Options dialog box activated by the **General...** menu command in the **Options** menu. To change the active database all files including designs and materials must first be closed. Then the Materials Folder selection box will be unlocked and either a database in the list chosen or a new one entered by clicking the **Browse** button and using the **Make New Folder** button when an appropriate location has been selected. If a new folder is created and a corresponding database does not exist then the option of creating a new database is given. This will be an empty database except for one material, Air, and one substrate Lossless

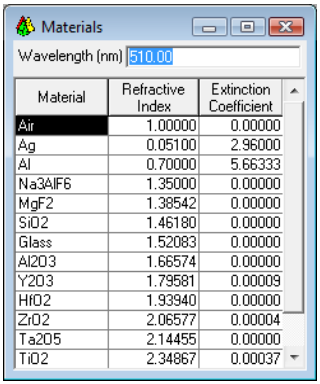
The **Maintain Folders** button allows you to control the display order of the materials databases, add new databases and remove databases from the list. Removing a database from the list does not delete the database from your computer. Clicking the Maintain Folders button displays the dialog below:



Click the Add button to add a new materials database to the list. The new database will be added to the bottom of the list. Select a database by clicking on it and the click Edit to change the materials database. This will replace the database in the list with the new database. With a database selected, use Move Up and Move Down to change its position in the list. Clicking the Remove button will remove the database from the list. Note that the current materials database is not displayed in this list.

Displaying list of materials in database

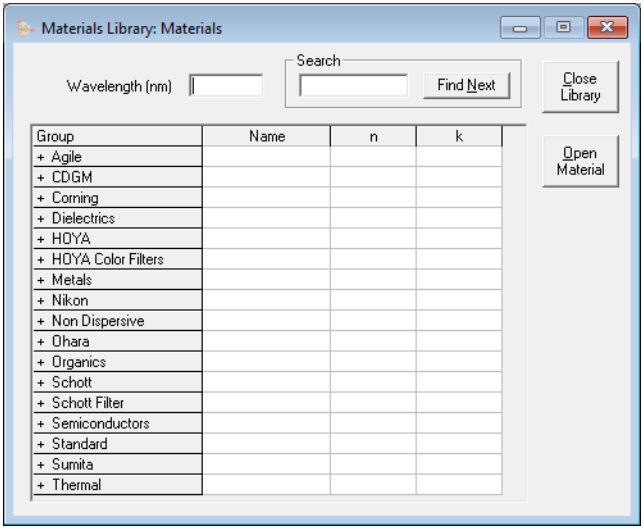
The **Tools** menu for most windows carries the item **Materials**. This activates a list of materials that are in the database together with their optical constants at the wavelength specified at the top of the table. To change the wavelength, edit the value in its cell at the top of the table.



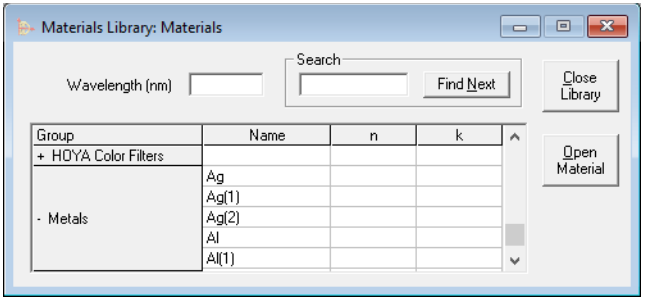
The order of the materials in the table is identical to that in the popup lists in design tables. This order can be changed. The **Sort** option under **Edit** offers criteria under which the entire list can be ordered. Alternatively, to move a material name individually, click once in the box containing it then use the mouse to drag the name to its new position. If the name is dragged out of the current limits of the table then no change will be made.

Importing materials from the Materials Library

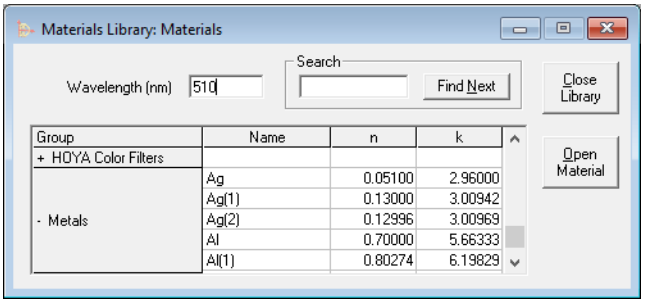
The Essential Macleod is supplied with a Materials Library. The Materials Library is a collection of material data organized by groups (for example, metals, dielectrics) but is displayed in a single hierarchical list format. To open the materials library, select **Browse Materials Library…** in the **Tools** menu.



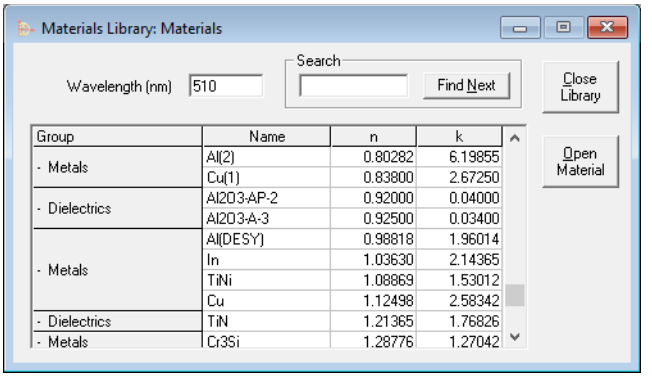
A newly opened materials library window appears as above. The materials in the library are contained in several groups. Double-click on a group name to show the members of the group.



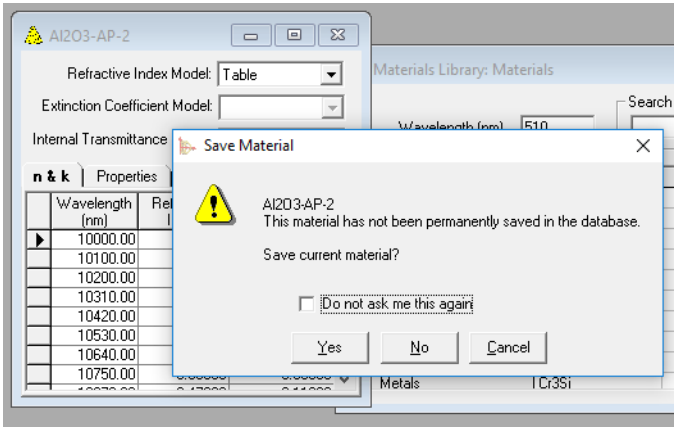
Here, the first few members of the Metals group are visible. Refractive index information is not displayed because a wavelength has not been entered. Enter a wavelength value into the wavelength box and press **<Enter>**.



Refractive index values will appear for the entered wavelength. You can open more than group at a time. Double-click on another group name and its members will also appear. Double-clicking on a group name that has its members displayed will close that group. The materials can be sorted in different orders. Double-clicking in a header will first sort the list into ascending order for that header. Double-clicking again in the same header will change the sort into descending order. Here a part of the Metals and Dielectrics groups has been sorted into order of ascending n.



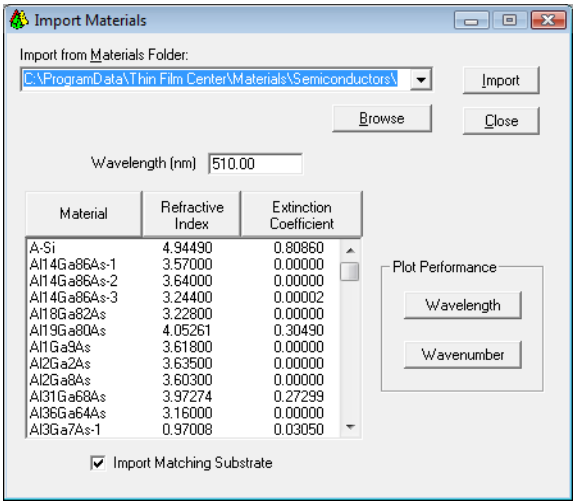
To load a material from the library into the current materials database, you can either double-click on the material name, or select the material name and click the **Open** button. If a material of the same name does not already exist in the materials database, then material will be opened and given the same name as in the library. If the material name already exists in the materials database, then the material name will be opened and given a modified name that does not already exist in the database. Where available, the library also contains internal transmittance data in the material definitions. When materials are opened from the library, they have a temporary status. They can be used in designs etc. but they are not permanently saved in the materials database. Closing a material without saving it will cause the material to be deleted after the last item using it is closed. If you close the material before it is saved, you will receive a warning about the temporary status of the material.



Importing materials from another database

To import materials from other databases, first use the **Materials** command in the **Tools** menu to activate the Materials window where the materials list is displayed. Then use the **Import** command in the **Edit** menu. The materials database from which materials are being copied is selected in the usual dropdown list. Multiple materials, including

noncontiguous ones, can be selected by clicking on them. To deselect a material click on it again. This makes it very easy to create a new materials database for a new project, particularly useful when some changes in the system of units are expected, such as moving to the infrared and working in terms of microns instead of nanometres.



Should a material be selected for import that exists already in the active database then a dialog box appears asking if the current material should be overwritten. If the answer is negative then a further dialog asks for a new name for the material. The operation can be canceled at this stage.

The materials database dropdown list has a limited capacity. Should the database from which the materials are to be imported not be in this list, its path and name can simply be typed into the database field. The **Browse** button can also be used to display a folder browser. The material database can be selected from the list of folders. As soon as it has been correctly entered, the materials from it appear in the scrolling selection list. If this does not happen and it appears impossible to leave the database field, then it is an indication that the path or database name as entered is incorrect. Although a final backslash is shown in the diagram, it is optional.

The list of materials also shows the optical constants for the material at the wavelength specified above the list. This wavelength can be changed if desired. After entering the wavelength, press the <Enter> key or click in another box to update the optical constants. You can also plot the optical constants against wavelength or wavenumber (frequency) in the current units by clicking the **Wavelength** or **Wavenumber** buttons.

To support older materials databases where substrate data is kept is separate files, if **Import Matching Substrate** is checked before materials are imported, then substrate definitions with the same names as the materials will also be imported into the current materials database.

Exporting and Importing Individual Materials

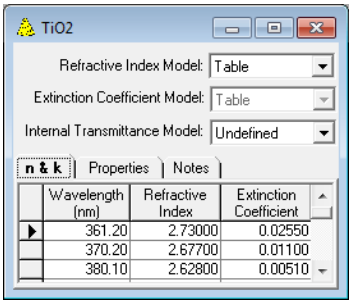
Individual materials may be exported from one copy of the Essential Macleod and imported by another copy. To export a material for import by another copy of the Essential Macleod, open the material either by using the **Open Material…** command in the **File** menu, or by double-clicking on the material name in the Materials window (**Tools** menu -> **Materials**). From the **File** menu, select **Export** and then **Material**. You will be prompted to choose a filename and location to store the data. The filetype for exported material data is "mtx". This is a text file and may easily be sent as an attachment to an email.

To import a material in an mtx file into the current database, you can either drag-and-drop the mtx file onto the Essential Macleod desktop, or you can use **Open** in the **File** menu. Set the filter to All files (*.*). If there are many files in the folder, you can type *.mtx into the filename box to show only the mtx files. Open the mtx file and the data will be loaded into a new material window. If a material of the same name does not already exist in the materials database, then material will be opened and given the same name as in the source copy of the Essential Macleod. If the material name already exists in the materials database, then the material name will be opened and given a modified name that does not already exist in the database. The new material will have a temporary status. It can be used in designs etc. but it is not permanently saved in the materials database. Closing the material without saving it will cause the material to be deleted after the last item using it is closed. If you close the material before it is saved, you will receive a warning about the temporary status of the material.

Display of Materials Data

The material data can be displayed simply by using the **Open Material...** command under the **File** menu. An alternative is to double-click the material name in the materials list displayed by the **Materials** command in the **Tools** menu. This displays material data in a material window. Once the material window is active, the **Plot** menu permits the plotting of optical constants against wavelength or frequency.

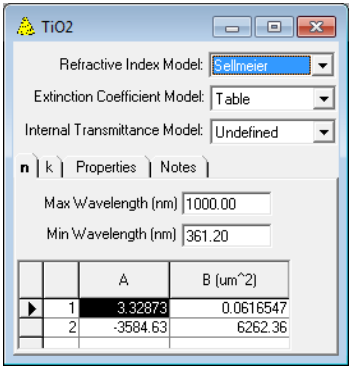
The data displayed depend upon the model being used. For refractive index there are several possible models: **Cauchy**, **Sellmeier**, **Table, Drude, Lorentz, Drude-Lorentz** and **Hartmann**. For extinction coefficient, there are four possible models: **k = 0**, **Table, Cauchy** and **Exponential**. When the refractive index model is **Table**, the extinction coefficient model is always **Table**. The models to be used are selected by the drop down lists at the top of the Material window.



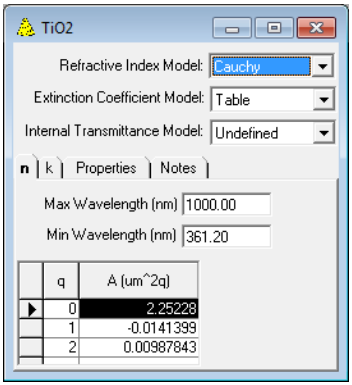
For the non-tabular models (see below), the parameters are supplemented with increments. These increments are only used by Reverse Engineer.

For Table data, the refractive index and extinction coefficient are entered as triplets of wavelength, refractive index and extinction coefficient. Values in between the wavelengths are derived using linear interpolation. For wavelengths less than the first value or greater than the last value, the first and last values are used respectively.

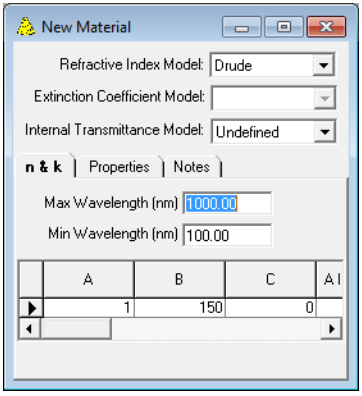
For Sellmeier data, the A and B parameters are entered as pairs, one pair for each term in the model. A minimum of one term must be entered. The number of terms available is essentially unlimited. In addition to the terms, the wavelength limits must also be specified. For wavelengths less than the minimum wavelength or greater than the maximum wavelength, the refractive index at the minimum wavelength and the refractive index at the maximum wavelength are used respectively.



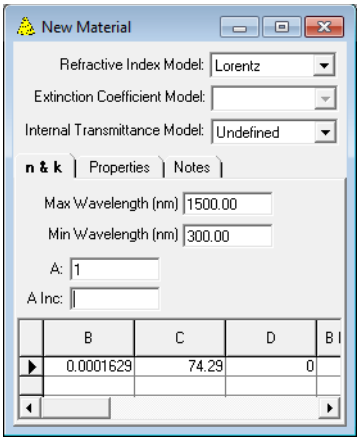
For Cauchy data, the A parameters are entered for each q. A minimum of one term must be entered. The number of terms available is essentially unlimited. In addition to the terms, the wavelength limits must also be specified. For wavelengths less than the minimum wavelength or greater than the maximum wavelength, the refractive index at the minimum wavelength and the refractive index at the maximum wavelength are used respectively.



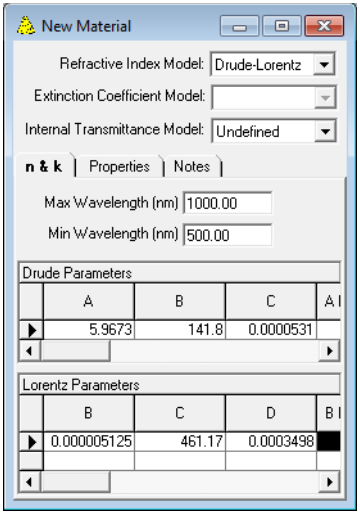
For the Drude model, there are just three parameters, A, B and C. Wavelength limits must also be entered.



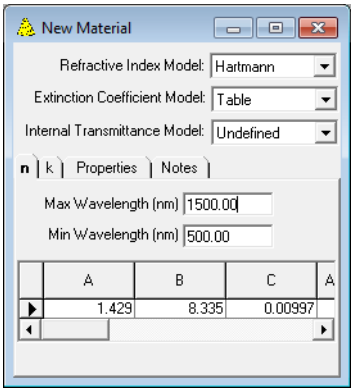
For the Lorentz model, each oscillator can be entered on a single row. The single oscillator model below is representative of MgF_2:



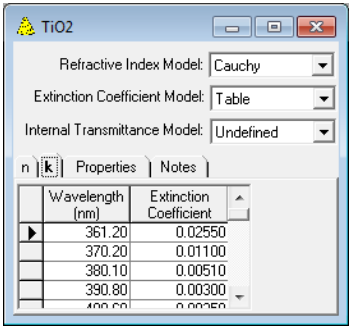
In the case of the Drude-Lorentz model, both the Drude and Lorentz components are entered. The model below is representative of gold:



For the Hartmann model, there are just three parameters, A, B and C. Wavelength limits must also be entered. The coefficients below represent SiO_2.



For tabular extinction coefficient data associated with a Sellmeier or Cauchy model, the extinction coefficient data are entered as pairs of wavelength and extinction coefficient values. Values in between the wavelengths are derived using linear interpolation. For wavelengths less than the first value or greater than the last value, the first and last values are used respectively



Manual Entry

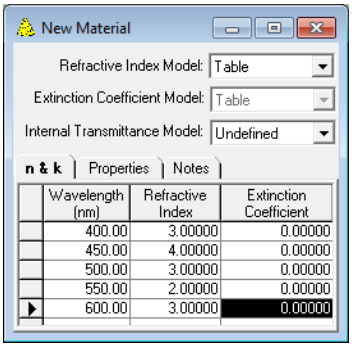
Entry of new information or editing of existing values can readily be performed in the same way as with any other table of parameters. Data can also be pasted in from the clipboard. The operation of the insertion command for tabular refractive index data is a little different from other parameter tables and will now be described in greater detail.

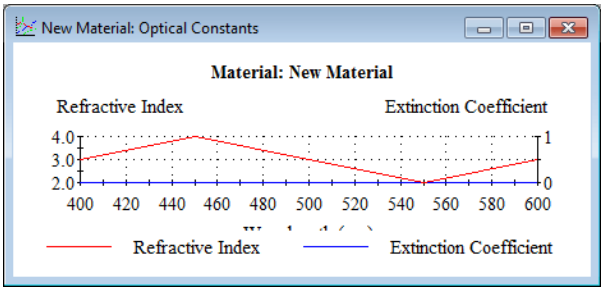
Insert Points for Tabular Data

In the calculations throughout the package, whenever values of the optical constants are required at wavelengths for which there is no entry in the table, they are linearly interpolated from the existing data. Any other form of interpolation requires values beyond the nearest wavelength points in the table. It may be that a more involved form of interpolation is appropriate in particular cases where there is a sudden change in the sense of variation of the optical constants. This is the purpose of the special insertion command for optical constant data. It uses a cubic spline interpolation procedure that operates on

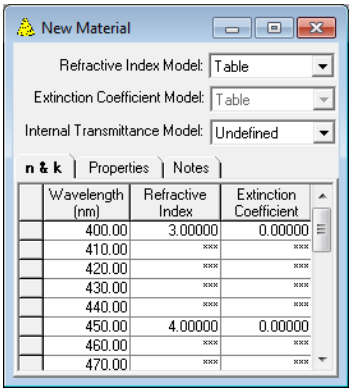
the entire data table. If, therefore, there is a gap in a table where the sudden changes in optical constants suggest that linear interpolation would not be the best form then the gap may be filled in using the cubic spline method and the results stored in the material table. Then the calculations will simply linearly interpolate these new values and any problems are completely avoided but the speed advantages of linear interpolation are retained.

We can illustrate this by an example, admittedly contrived. The following table shows a set of refractive index values against wavelength. They oscillate sharply between 2 and 4 and the plot of the refractive index values in the following diagram shows very sharp peaks and troughs.



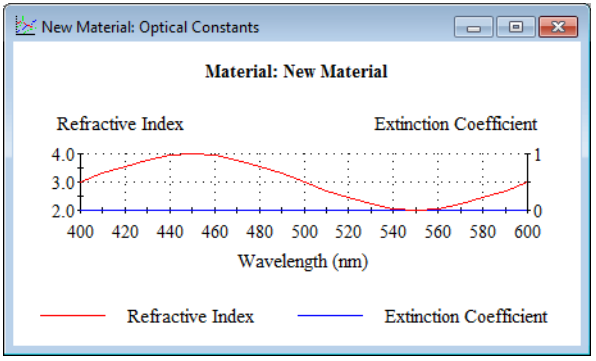


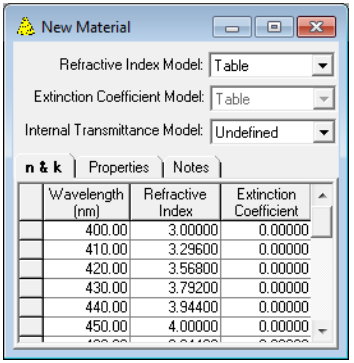
In the table we now insert four points between each of the primary wavelengths. The resulting table has the appearance shown in the next figure.



Wavelengths have been inserted but the inserted refractive index and extinction coefficients are indicated by asterisks showing that the corresponding values will be determined by a cubic spline interpolation once the window is closed or whenever a plot is required. Values can however be manually entered into any of the cells with asterisks and will be treated as valid data.

Now we select **Plot** and **Plot on Wavelength Scale** from the menu. The plot that appears is given in the next figure followed by the new table of values.





Wavelength Scale...

Materials data are held in generic units (actually nanometres) and converted automatically to whatever display units are in force. There is therefore normally no need to alter the wavelength scale of a material. However, there may be occasions when it is realized that a material wavelength scale is off in some respect. Maybe it was entered incorrectly or has not been properly converted from a database of an earlier type. If the data for entry is of a different scale it is nevertheless often convenient to enter it first and then to make any necessary corrections. This is the purpose of the **Wavelength Scale...** menu item. The **Wavelength Scale...** command is only available when the **Refractive Index Model** is **Table**.

The option should be used with caution. It asks for the **Wavelength Units of This Material**. If the material has just been entered then the wavelength units box should have the Scale Factor for the current material wavelength scale. If the units are microns, for example, then the number entered in the box should be 1E-06. If the material has been entered previously and it is only now realized that the wavelength scale is incorrect then it may be a more complicated operation because the wavelength scale may not now be that originally entered. Examine the current wavelength entries. Decide on the factor that must be used to convert them into correct values. For example, if the wavelength value shown in the table is 1000 and the correct value should be 1.0, then the conversion factor is 10^{-3}. Write down the scale factor for the correct current wavelength units. If the current scale units are microns then the scale factor is 1E-06 or 10^{-6}. Multiply this scale factor by the conversion factor to give the number that must be entered in the dialog box. In the present example this will be $10^{-3}\times10^{-6}=10^{-9}$ or 1E-09.

Should it happen that all the materials in a database are incorrect by the same factor then correction on an individual basis can become exceedingly tedious. In such a case it is better to scrap the units definition file. First calculate the necessary scale factor as detailed above. Make a note also of the various units in the General Units box. Close the Essential Macleod. Find the folder with the relevant materials database. Rename the file **Units.tfp** to **Units.tmp**. Open the Essential Macleod and enter the universal correction factor, calculated as in the previous paragraph, You will need also to reenter the general units. Check that all is well and if so then dispose of the file **Units.tmp**.

Packing Density...

The refractive index of a thin film depends not only on the material but also on the packing density. Even if two films were constructed from exactly the same material, their refractive indices would be different if their packing densities were different. Thin films rarely have the same refractive index as similar bulk materials, for example. This menu item allows the indices of a stored material to be altered as though the packing density had changed. It is useful in, for example, the correction of bulk material values more closely to agree with what might be expected from a thin film. It can also be used to adjust the material constants in an alternative database to represent materials deposited at a different substrate temperature. The model used for the relationship between index and packing density is discussed in greater detail earlier in this manual. It is a linear one simply because many materials have been shown empirically to obey a linear law. The dialog box that appears asks for a new value of packing density. This value assumes that

the current packing density is unity. Alternatively, since the law is linear, the entry is equivalent also to a proportional change in packing density. For example an entry of 0.9 followed later by an entry of 1/0.9=1.111111 will restore the indices to their original values. The **Packing Density …** command is only available when the **Refractive Index Model** is **Table**.

Exercise caution in the use of this command. Once the change has been made there is no indication that the values are anything other than normal. The command should not be used unless it is very clear and unmistakable that the material is now different from standard. Thus the name of the database should reflect the situation or the name of the material should be changed in some way.

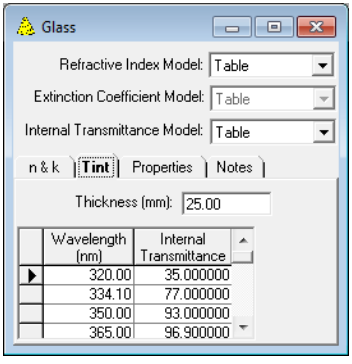
Internal Transmittance Data

Internal transmittance is described in greater detail in the Stack chapter of the manual. Briefly it is used in the calculation of transmittance through a thick medium in a Stack or in a Design. Extinction coefficient, *k*, is often very small and not known with sufficient precision for reliable calculations of thick material properties, and internal transmittance, the parameter usually published by material suppliers, is safer.

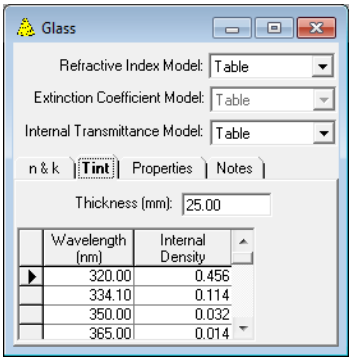
Previously internal transmittance was published in separate substrate files but is now incorporated in the material files along with the *n* and *k* values. To reveal the Substrate menu items, now not present by default, use the **Legacy** tab in the General Options dialog, accessible through **General...** in the Options menu.

The Internal Transmittance Model field in the Material document presents four choices, **Undefined**, **Lossless**, **Table** and **Use k**. Undefined means that there is no internal transmittance data in the Material file and if a legacy substrate file exists it should be used. Lossless means that the internal transmittance is 100% for all wavelengths. Table means that internal transmittance is specified as a table of values against wavelength. Use k means that internal transmittance values will be derived from the extinction coefficient values. This method is not recommended but is provided for use where no other information exists and the *k* values are considered reliable.

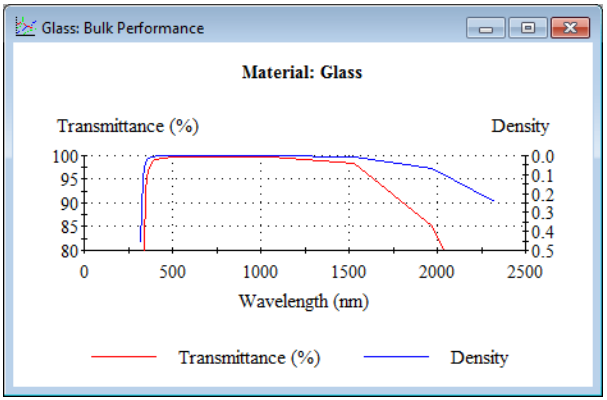
Tabular data can only be entered when the Internal Transmittance Model is set to Table and the Tint tab has been selected. Also under this condition any existing Substrate document can be copied and pasted into the Material document.



It is possible to change the display to one of optical density against wavelength by selecting **Density Display** in the **Edit** menu. Again the optical density corresponds to internal transmittance. It does not include any reflection losses at the interfaces. To restore the transmittance select **Transmittance Display** in the **Edit** menu.



The substrate data can readily be plotted. Select the appropriate option from the **Plot** menu.



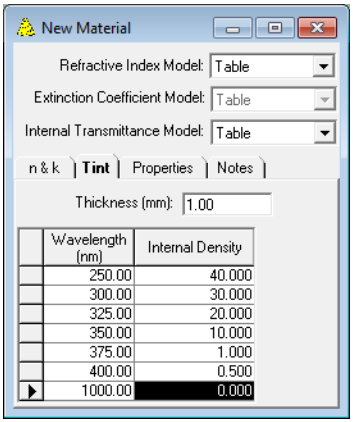
The graphs are, like those from tables, plotted initially with scales that are taken from the maximum and minimum values in the table. To change these the plot window should be active and then **Parameters...** in the **Edit** menu should be selected.

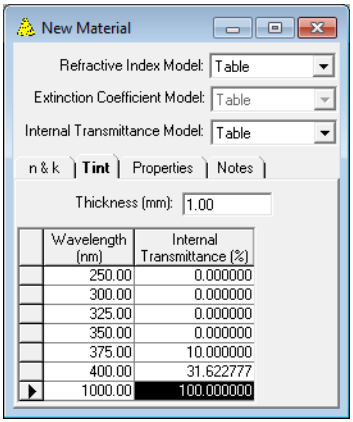
Editing the internal transmittance data is quite similar to the editing of the refractive index data but there are some slight differences. Since density and transmittance are directly related analytically they cannot be entered independently. Therefore the display shows either transmittance or density but not both together.

There are many different types of interpolation that could be used for calculating the inserted values but the great range of values, sometimes many orders of magnitude, leads to unsatisfactory performance. Polynomial and spline interpolation although they give nicely smoothed curves have a pronounced tendency under such circumstances to

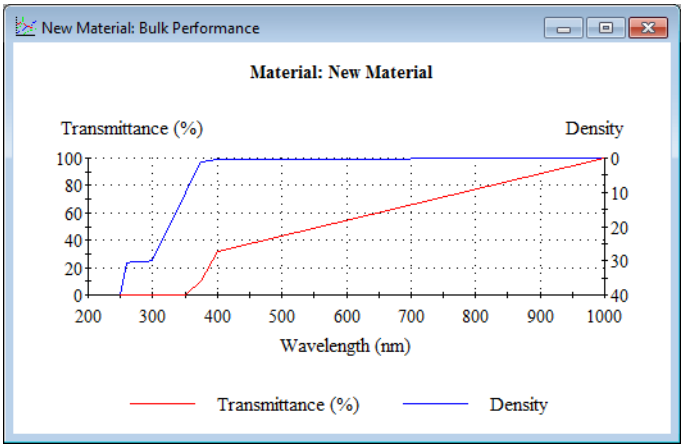
produce spurious peaks and these peaks can often exceed 100% transmittance or take negative values. The insertion of values in this editor, therefore, is accomplished by linear interpolation. Values can then be adjusted manually if they appear to need it. When points are inserted the transmittance and density values are not calculated. Instead a series of asterisks, ***, is shown. These can be replaced by manually inserted values if desired. Linear interpolation of any values that are still represented by asterisks will take place if a plot is initiated or if the substrate is saved. The interpolation will be in terms of the particular parameter that is currently being displayed.

Linear interpolation, however, can also lead to difficulties when there are wide differences at the ends of the interval. We illustrate this by a notional substrate file. We constructed this by inserting the density figures. The corresponding transmittances are shown on the right.

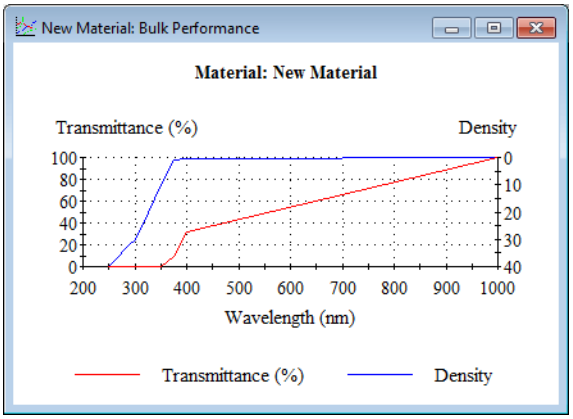




Now we insert four points between 250 and 300, first making sure that transmittance is displayed. We insert the rows and the new transmittance values are shown simply as a set of asterisks. Next we trigger the interpolation by selecting a plot. The asterisks change to the interpolated values that are simply shown as zero transmittance. In terms of density, however, we see that there is a rather unrealistic plateau on the curve.



Under such circumstances it is better to interpolate so that the density values form a linear progression. We can do that by deleting those we have just entered and switching to density before interpolating. The resulting linear progression in density corresponds to an exponential increase in transmittance that appears much more realistic.

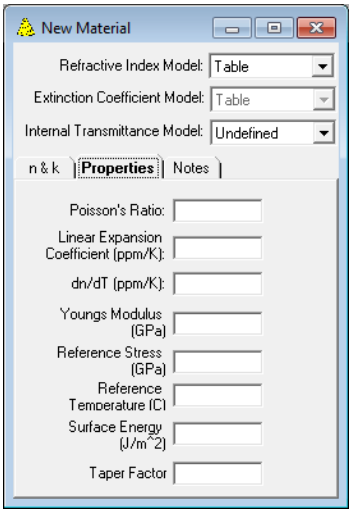


Inserting values, therefore, is a linear interpolation process. The linear values will be in terms of transmittance if it is transmittance that is displayed, or density if density is displayed. In most cases transmittance is better if the values are high so that the material is fairly transparent. Density is better if transmittance is low and especially if there are order of magnitude changes. For intermediate values some experimentation may be required. This type of interpolation is preferable to, and avoids the problems inherent in, other forms.

Once the editing has been completed, we can save the revised data either as a new material or as a modification to the original by selecting **Save** or **Save As...** from the **File** menu.

Thermal Model

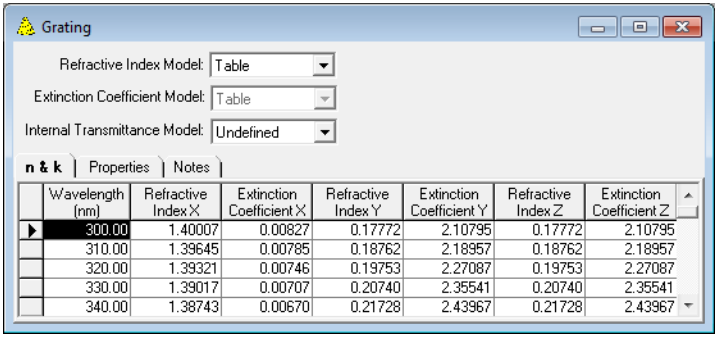
To enter the thermal properties for a material, click on the Properties tab.



The three thermal parameters for the material can then be entered in the top three boxes. The units for the Linear Expansion Coefficient and dn/dT are fixed. The parameters after the three thermal parameters are used by the stress model (see page 243) and the uniformity model (see page 24)

Birefringent Materials

The default material window allows entry of optical constant data for isotropic materials. Select **Birefringent** from the **Edit** menu to change the material display to the birefringent data form.



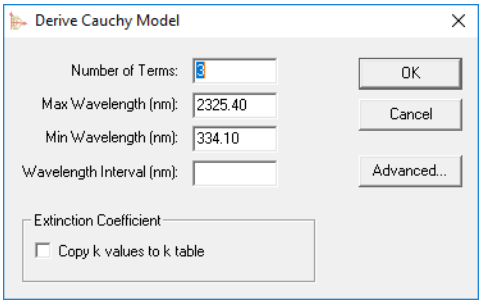
Wavelength (nm)	Refractive Index X	Extinction Coefficient X	Refractive Index Y	Extinction Coefficient Y	Refractive Index Z	Extinction Coefficient Z
300.00	1.40007	0.00827	0.17772	2.10795	0.17772	2.10795
310.00	1.39645	0.00785	0.18762	2.18957	0.18762	2.18957
320.00	1.39321	0.00746	0.19753	2.27087	0.19753	2.27087
330.00	1.39017	0.00707	0.20740	2.35541	0.20740	2.35541
340.00	1.38743	0.00670	0.21728	2.43967	0.21728	2.43967

For birefringent materials, optical constants for each of the three principal axes are required. The three principal axes are labeled x, y and z. The x axis is parallel to the

surface of the films and parallel to the plane of incidence. The y axis is parallel to the surface of the films and normal to the plane of incidence. The z axis is normal to the surface of the films.

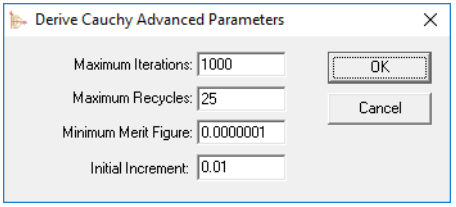
Generating Refractive Index Models

Sellmeier and Cauchy terms can be derived from tabular data. This is performed through the **Derive Cauchy…** and **Derive Sellmeier…** commands in the **Edit** menu. **Selecting Derive Cauchy…** displays the following dialog.



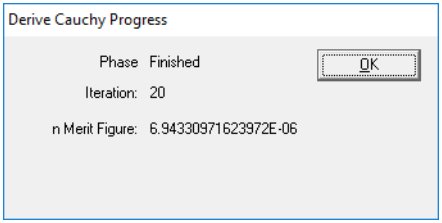
Number of Terms specifies the number of terms in the derived model. The **Max Wavelength** and **Min Wavelength** specify the limits of the data to be used in the derivation. By default, these encompass the entire data in the Material table, Where the wavelength is very broad and includes, for example, resonances, it may be necessary to restrict the wavelength range to the part of the data where the refractive index dispersion is well-behaved otherwise a good fit will not be achieved. **Wavelength Interval** specifies a sample interval to be used on the tabular data. By default this is blank and this means use the data points in the table without sampling. If a value is entered, the data are re-sampled using the specified interval by linear interpolation. Re-sampling may be necessary to improve the fit in regions where there are relatively few data points, for example, a region where the dispersion is relatively linear. In the **Extinction Coefficient** box, you can choose to **Copy k values to k table**. If checked, the k values associated with the tabular refractive index values will be copied to the extinction coefficient table for use with the Cauchy model.

Clicking the **Advanced…** button will display more parameters associated with the derivation.

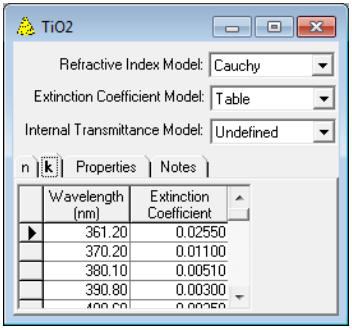


The derivation uses non-linear simplex optimization to fit the model to the tabular data. These are parameters that control the Simplex optimization and have same meaning as in Refinement. Generally, these parameters will not need to be altered.

Clicking **OK** in the Derive Cauchy Model dialog will start the derivation. A progress window will appear and at the finish of derivation it will show the Phase as Finished and also show the final merit figure. This is the rms deviation of the model from the (possibly re-sampled) data points. Smaller numbers indicate a better fit.

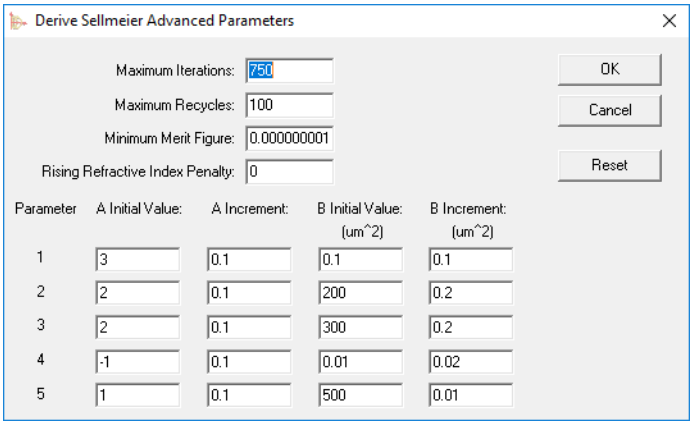


Click **OK** to complete the derivation process. To see the results, select **Cauchy** in the **Refractive Index Model** list in the Material window.



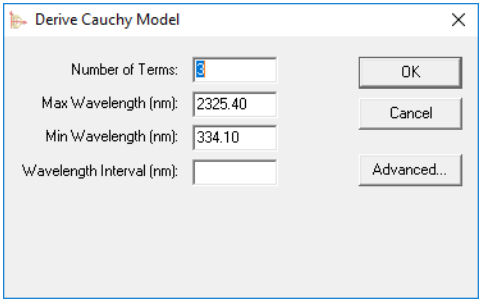
If **Copy k values to k table** was checked in the **Extinction Coefficient** box, then make sure that the **Extinction Coefficient Model** is set to **Table**. To keep the model data and use it in future calculations, save the Material. The original tabular data are not deleted, it is simple to return to using the tabular data by simply changing the **Refractive Index Model** back to **Table** and saving the Material.

The Sellmeier derivation proceeds in a similar manner. The difference between the Cauchy and Sellmeier derivation is in the advanced parameters. For most materials the starting values shown below work well, however, for more unusual materials, these parameters may not result in a good fit and the fit might be improved by modifying the starting values.



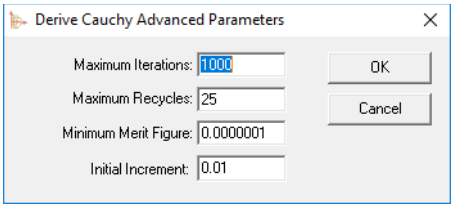
Generating Extinction Coefficient Models

Cauchy and Exponential terms can be derived from tabular data. This is performed through the **Derive Cauchy (k)…** and **Derive Exponential (k)…** commands in the **Edit** menu. Selecting **Derive Cauchy (k)…** displays the following dialog.



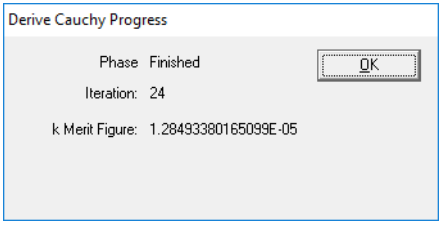
Number of Terms specifies the number of terms in the derived model. The **Max Wavelength** and **Min Wavelength** specify the limits of the data to be used in the derivation. By default, these encompass the entire data in the Material table, Where the wavelength is very broad and includes, for example, resonances, it may be necessary to restrict the wavelength range to the part of the data where the extinction coefficient dispersion is well-behaved otherwise a good fit will not be achieved. **Wavelength Interval** specifies a sample interval to be used on the tabular data. By default this is blank and this means use the data points in the table without sampling. If a value is entered, the data are re-sampled using the specified interval by linear interpolation. Re-sampling may be necessary to improve the fit in regions where there are relatively few data points, for example, a region where the dispersion is relatively linear.

Clicking the **Advanced…** button will display more parameters associated with the derivation.

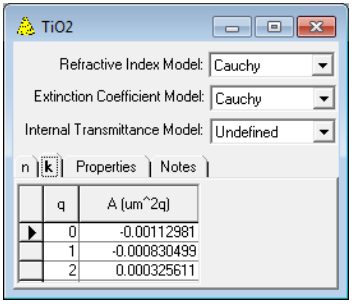


The derivation uses non-linear simplex optimization to fit the model to the tabular data. These are parameters that control the Simplex optimization and have same meaning as in Refinement. Generally, these parameters will not need to be altered.

Clicking **OK** in the Derive Cauchy Model dialog will start the derivation. A progress window will appear and at the finish of derivation it will show the Phase as Finished and also show the final merit figure. This is the rms deviation of the model from the (possibly re-sampled) data points. Smaller numbers indicate a better fit.



Click **OK** to complete the derivation process. To see the results, select **Cauchy** in the **Extinction Coefficient Model** list in the Material window, after changing the **Refractive Index Model** from **Table**.

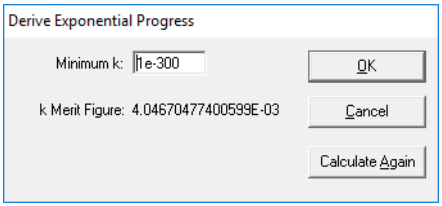


To keep the model data and use it in future calculations, save the Material. The original tabular data are not deleted, it is simple to return to using the tabular data by simply changing the **Refractive Index Model** back to **Table** and saving the Material.

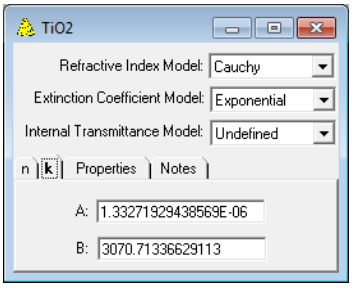
The exponential model used is:

$$k(\lambda) = Ae^{B/\lambda}$$

A and *B* are determined by a least squares fit of the exponential model to the k data. To aid the fitting process and avoid problems where the k value is zero, a minimum k value can be set. Values of k less than this value are not used in the calculation. Selecting **Derive Exponential (k)…** causes a fit to be performed to the data and the rms difference is displayed.



If the fit is not satisfactory, changing the **Minimum k** value might improve the fit. After changing the value, click **Calculate Again** to recalculate the A and B parameters. Click **OK** to copy the parameters to the Material window. To see the results, select **Exponential** in the **Extinction Coefficient Model** list in the Material window, after changing the **Refractive Index Model** from **Table**.



Deleting Materials

Deleting a material is discouraged because of future compatibility problems when reading a design that may have used that material. It is far better just to create a new material database and import the materials with the exception of the one that is to be removed. However there may be occasions when deleting a material is necessary.

First the menu item Materials under the Tools menu should be selected which presents the materials window with the list of materials in the current database. Select the material that you wish to delete by clicking on the name, then select **Delete** in the Edit menu. If you need to recover a deleted material, select **Undelete** in the Edit menu. A window will appear listing the deleted materials in the database. Select the materials that you wish to restore and click **Undelete**. The materials database will recycle deleted materials. If you have added materials to the database since deleting a material, it may not be possible to recover the deleted material.

We emphasize once again that the best practice is never to make alterations except adding new materials to an existing materials database. This preserves compatibility with all previous designs that have used that particular database. If changes other than additions of materials are to be made then it is better to create a new database, to copy only the desired materials from the existing one to it and then to make any alterations before creating any designs. This preserves integrity. It is fairly easy to devise a naming convention that keeps track of what is happening. The designs, too, should be kept in separate design folders or even in the appropriate materials folder. Archiving is then a simple matter.

Optical Constant Extraction

Optical constants can be extracted from reflectance and transmittance data using a variant of the envelope technique. The films should be essentially dielectric with thicknesses such that there are extrema within the wavelength range of interest. Absorption may be included provided that it is not so great that the fringes are washed out. The films may also be inhomogeneous provided that the variation of index through the film is monotonic and the index contrast at the boundaries between film and surrounding media is larger than the inhomogeneity.

The technique used is of the class known as envelope methods. Such methods focus on the maxima and minima of reflectance and/or transmittance and the first stage of the calculation involves the interpolation of the maxima and minima to generate the envelopes. The ideal envelopes consist of the substrate transmittance or reflectance and the ideal quarterwave transmittance or reflectance. When the layer is absorbing, or inhomogeneous, the maxima and minima depart from these ideal envelopes by an amount that increases with thickness but, when absorption and/or inhomogeneity is not too high, the envelopes can still serve to launch the n and k calculations. An advantage of the method is that layer thickness is not, initially, required. It is calculated later in the process. The Essential Macleod technique gives a best fit to the level of the extrema but the technique concentrates on the level rather than position of the extrema in the first instance. This avoids the major discontinuities that can occur in other techniques. The variation of absorption in the film with wavelength is determined but at first in terms of a parameter that contains extinction coefficient and thickness together. Once thickness has been determined then a value can be placed on the extinction coefficient. Films are often inhomogeneous and so the method includes the possibility of inhomogeneous films. The technique, like all others, does have multiple solutions and has to ensure that the correct one is adopted. This means reducing the range that is searched by giving additional information. First, the user is asked to identify each extremum as a quarterwave or a halfwave condition. This reduces the number of solutions for a weakly absorbing film to two. Then the user is asked to give a rough estimate of film index. The solution nearest to this estimate is chosen.

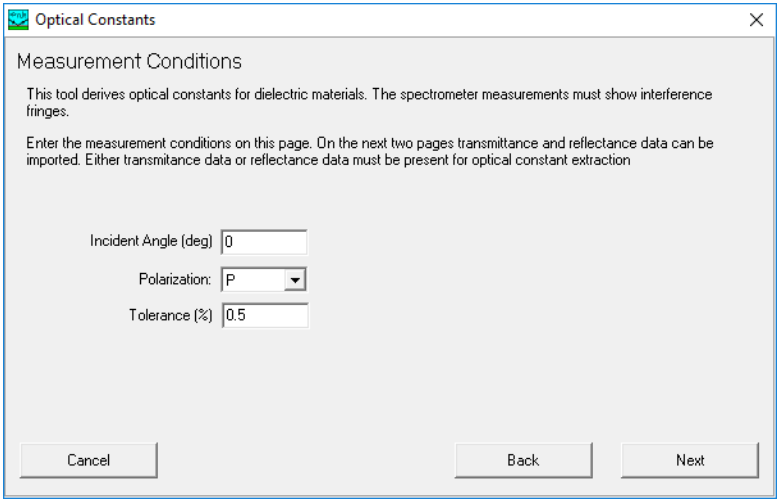
If the positions of the extrema are accurately determined then they do give useful information about the dispersion of the optical constants although they tell nothing about the absolute levels. We can choose to accept the absolute level determined by the envelopes and correct the dispersion to agree with the extrema positions. This can be useful, for example, when there are problems with noise or absolute accuracy over part of the region concerned.

The particular method has been compared with others in common use and was chosen over them because of its great stability. In many methods, errors committed in the determination of the reflectance and/or transmittance figures can have serious consequences for the extracted optical constants, sometimes making it impossible to derive physically possible results at all. Of course measurement errors will lead to optical constant errors because it is impossible to derive exactly correct results from incorrect measurements, but the consequences of errors can be magnified enormously in the derived results. Such magnification is largely avoided by the method adopted here.

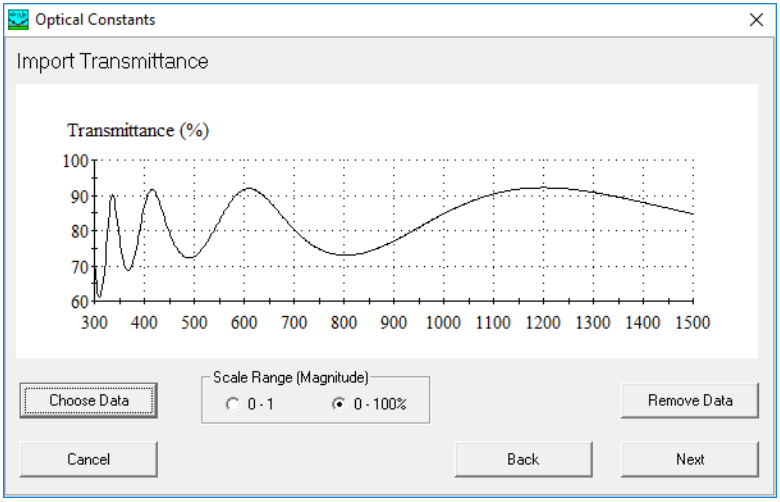
The input consists of the maxima and minima of transmittance and/or reflectance. For transmittance data, the measurement must be taken with an uncoated rear surface and include the multiple reflections generated by the rear surface. The reflectance measurement may be made under the same conditions, or the rear surface may be treated so that the reflections from the rear surface are eliminated. There are tools to assist in extraction of the necessary data from raw spectrometer records described later.

Accuracy estimates for the input should be provided and will be used by the program to modify the results if a good fit cannot otherwise be obtained. Two possible results usually exist and that nearest the estimated value of film index will be accepted. When measurements are transmittance only then either an inhomogeneous non-absorbing model or a homogeneous absorbing model may be chosen. Reflectance only results use an inhomogeneous non-absorbing model and reflectance and transmittance results use an inhomogeneous and absorbing model. Extrema wavelengths are not usually fitted exactly but the reflectance or transmittance figures are matched as well as possible and then the thickness is chosen for best fit wavelengths. If the extrema wavelengths are judged most important an option that first fits the reflectance or transmittance figures and then alters the optical constants to fit the wavelengths of the extrema may be selected. Note that the positions of the extrema influence the dispersion of the indices rather than their absolute level.

To launch this extraction process select **Optical Constant** from the **New** submenu of the **File** menu. You will then be directed to enter the measurement data and the measurement conditions.



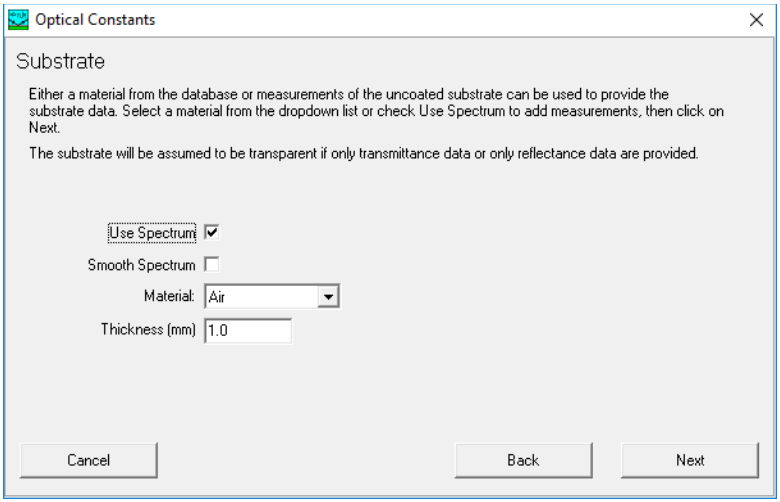
The first step is to enter the measurement conditions: **Incident Angle**, **Polarization** (when the incident angle is not zero) and **Tolerance** (the uncertainty in the measurement). Clicking **Next** then prompts you to import the transmittance data. This will be a measured spectrum in a text file. Click **Choose Data** to select the file. The Import Editor will be used so that you can define the data in the file.



When the file has been imported, a confirming plot will be displayed.

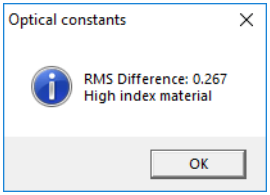
If you only have reflectance data, click **Next** without choosing any transmittance data.

Clicking **Next** prompts you to import reflectance data. The process is the same as for importing transmittance data. If you only have transmittance data, click **Next** to proceed to defining the substrate.

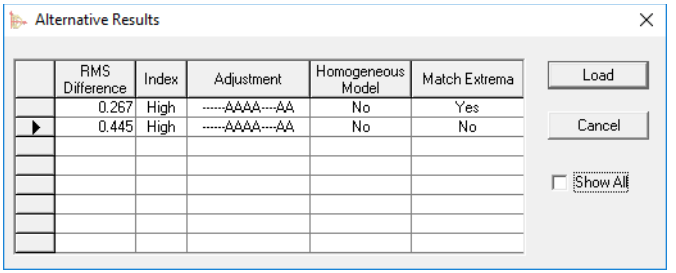


You can choose to either import a spectrum or use an existing material in the materials database. Clicking **Next** displays the Substrate Transmittance page. Here you can choose a transmittance data file or click **Next** to move to the Substrate Reflectance page. Here you can choose a reflectance data file. Both substrate transmittance and substrate reflectance data are imported in the same way as the film data. If you are using existing material data, click **Next** in both pages without choosing any data files.

After clicking **Next** in the Substrate Reflectance page, the software will automatically find the best set of parameters and present a summary.

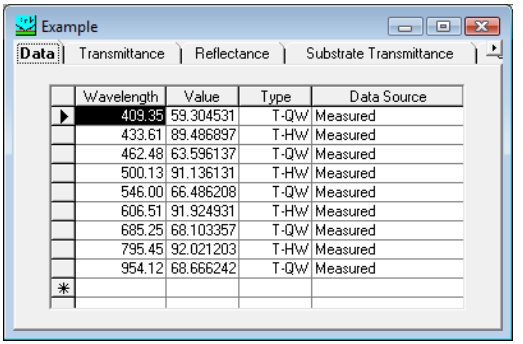


The RMS difference is between the imported data and the calculated performance using the extracted optical constants. The high/low index of the material is with respect to the substrate. A high index material has refractive index greater than the substrate. Clicking **OK** will present details of the results. This is the same as having selected **Extract n&k** in “The extraction process in operation” below. Alternate results are available by selecting **Show Alternatives** in the **Calculate** menu.



Each row lists an alternate solution. The Adjustment column indicates the number of data points that either needed adjustment or were flagged as bad results. To view an alternative result, select the row by clicking in the left cell and then click **Load**.

Clicking **Cancel** during the directed data entry will return you to an empty optical data window that has the general appearance of the following figure except that the columns will be empty. Note that this view of the data can always be activated by using the **Data** command in the **View** menu.



The menus corresponding to this window are similar to those for other windows with the exception of **View**, **Calculate** and **Create Material** and **Import** in the **File** menu.

The data window shows what will actually be used to carry out the calculations. The data consist of the maxima and minima of transmittance and/or reflectance *with no correction for the rear surface*, the only requirement is that the rear surface is uncoated. Maxima and minima are flagged as corresponding to quarter waves or half waves by the codes **T-QW**, **T-HW**, **R-QW** and **R-HW**. Substrate results can also be entered or they can be extracted from an existing material file (see below). These should be either uncoated transmittance results, flagged as **T-SUB,** uncoated reflectance results, flagged as **R-SUB**, or substrate refractive index, flagged as **N-SUB**. Either of two other flags must also be set for each input result. The column with the title **Data Source** can have either of two entries, **Measured** and **Envelope**. **Measured** corresponds to a real maximum or a minimum. **Envelope** indicates a result inserted simply to help the program draw the halfwave or quarterwave envelopes. These are interpolated by a cubic spline function and sometimes need a little help. Envelope results are intended for this. You will see the form of the envelopes when you use **Plot Performance** (see below) or are using

Transmittance or **Reflectance** in the **View** menu with **Show Envelopes** set. R and/or T results may be entered in any order. After the editor is closed the results are sorted into ascending wavelength.

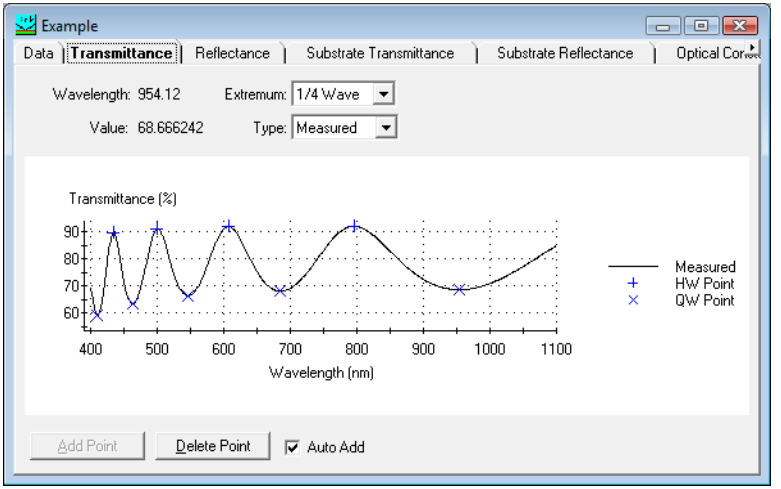
If only substrate transmittance data are provided, the substrate will be assumed free of absorption. Any actual transmission loss in the substrate will therefore be interpreted as lost by reflection at the interfaces and this implies a higher substrate refractive index. If substrate values are read from a material file then the extinction coefficient will be assumed to be zero.

Data Entry

Manual entry of the extrema is accomplished through the Data Window. Select **Data** in the **View** menu. The table can be edited in the normal way.

There will be many cases where the data are more involved or less suitable for manual entry. Then it is possible to import raw transmittance or reflectance versus wavelength data and there are powerful tools for extracting the information necessary for the calculations. Each data record should consist of a wavelength value and a value of transmittance or reflectance, delimited by either a space or tab character. The transmittance and/or reflectance scale should run either from 0 to 100% or from 0 to 1.0. Wavelength should be in the same units as those that are current. If this is not the case there are two options. If all data including substrate values are to be entered in this way then the wavelength scale can be adjusted later once the constants have been extracted. If, however, substrate values are to be taken from the current database then the general units must be changed to correspond with the data that are to be entered. Once the optical constants have been extracted then the general units can be reset.

The tabs **Transmittance** or **Reflectance** show a data display window. Initially this window is blank but the Import command in the File menu is now available and permits the importing of the reflectance or transmittance data into the window. A typical appearance of the window is shown below. Click on the mouse and drag a rectangle round one of the extrema on the curve. This defines a search region. Releasing the mouse button causes the peak to be located. Wavelength and value are then shown in the boxes at the top of the screen. Two other attributes of the extremum are required. One is whether the extremum corresponds to a quarterwave or a halfwave. The other is whether the point is to be treated as a measured point or an envelope point. Whenever possible, these entries will automatically be suggested, but the user must make sure that the entries are correct.



Once the details are verified, the **Add Point** button will transfer the data to the data window where it will be used for calculating the envelopes. The points identified as quarterwaves will be marked with a cross while the halfwaves are marked with a plus.

Envelope values give the user the capability of altering the shape of the envelopes. They are drawn by a cubic spline process and occasionally may need slight adjustment. Envelope points can be placed anywhere and are intended to help with the drawing of the envelope so that it is improved. They are used in the calculation just as any other point but are omitted from the procedure estimating film thickness. To create an envelope point anywhere on the diagram use **<Alt>** + **<Shift> <Left Mouse Button>**. The resulting symbol can be dragged to where it is wanted. Then the **Add Point** button will enter it as an envelope point.

Colors are used to help identify the various elements. Measured points are in blue, envelope points in red.

To check a point, select it by drawing a box round it. The top of the screen will show the appropriate values. To remove a point, first select it and when the values are confirmed use the **Delete Point** button.

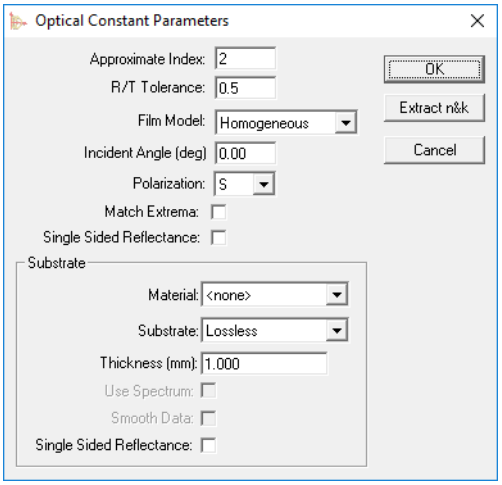
To change a point from envelope to measured and/or vice versa select it and then change the **Type** attribute by using the popup menu.

The Reflectance tab permits reflectance results to be entered and the Substrate Transmittance and Substrate Reflectance tabs allow substrate spectra to be imported and displayed. In these cases, no point identification is necessary. It will be automatic when the calculation is performed. The measured substrate data must include the rear surface reflections. This is necessary for the determination of the internal transmittance of the subsrtate.

Before the calculation is performed some parameters must be set. The **Parameters** command in the **Calculate** menu displays a dialog box that permits various quantities necessary for the extraction to be entered.

Approximate Index is required because of multiple solutions. Two possible indices usually exist and the program will select that nearer to the entered approximate value. If results that are clearly unlikely are obtained, then one of the first things to check is the entry under **Approximate Index**.

R/T Tolerance is to be given in percent and determines how the program will proceed if a valid solution cannot be obtained. The results will first be adjusted within the tolerance range (it is actually a little more complicated than that because it is a set of intermediate results derived from the input that are adjusted) and if a good solution is then achieved they will be flagged as **A** for adjusted. If even with adjustment a fit cannot be obtained then the results will be flagged as **B** for bad.



Film Model permits the choice either of a film model that is inhomogeneous and free of absorption or of a model that is homogeneous and absorbing. The choice is valid only when transmittance results are being interpreted. When the results are in reflectance only the option is ignored and the film model is always an inhomogeneous absorption-free film. When both reflectance and transmittance results are available the model is automatically set as inhomogeneous and absorbing.

Incident Angle specifies the incident angle of the spectrometer beam on the thin film being measured. All measurements must be conducted at the same incident angle. This allows the accuracy of the measurements to be improved when reflectance measurements are used. The maximum incident angle that can be used is 45 degrees.

Polarization specifies the polarization used for oblique measurements. Oblique measurements must be conducted with either s-polarized or p-polarized light. The same polarization must be used for all measurements.

Match Extrema needs some explanation. Under normal operation, extrema wavelengths are not usually fitted exactly but the reflectance or transmittance figures are matched as well as possible and then the thickness is chosen for best fit to the wavelengths. It may sometimes be that the extrema wavelengths are judged more reliable than the reflectance and transmittance figures. There is therefore an option that first fits

the reflectance or transmittance figures and then alters the optical constants to fit the wavelengths of the extrema. The positions of the extrema influence the dispersion of the indices rather than their absolute level and so the reflectance and/or transmittance figures are still important because they determine the level of the optical constants.

Substrate: Material allows substrate optical constants to be read from an existing materials file. The correct material should be selected from the list.

Substrate: Substrate allows the substrate internal transmittance to be read from an existing substrate file. The correct substrate should be selected from the list. This option is only available when the Material does not contain internal transmittance information.

When **Use Spectrum** is checked, the extraction will use the substrate transmittance (and reflectance if present) data in determining the film's optical constants. If **Use Spectrum** is not checked, the **Substrate: Material** and **Substrate: Substrate** information will be used in determining the film's optical constants.

Single Sided Reflectance. Frequently, monitoring chips that are used for monitoring in reflection are ground on the rear surface to eliminate its effect on reflectance measurements. This check box becomes available when reflectance measurements are present in the results and its selection removes the otherwise automatic rear surface correction from the calculations so that coatings deposited on reflection chips may be assessed.

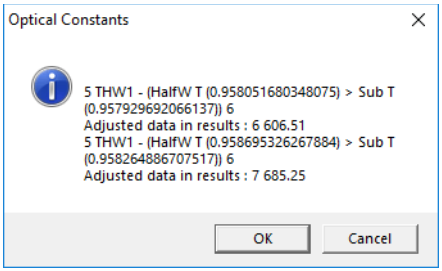
When **Smooth Data** is checked, the measured transmission data will be smoothed before values are extracted for used in optical constant determination.

The extraction process in operation

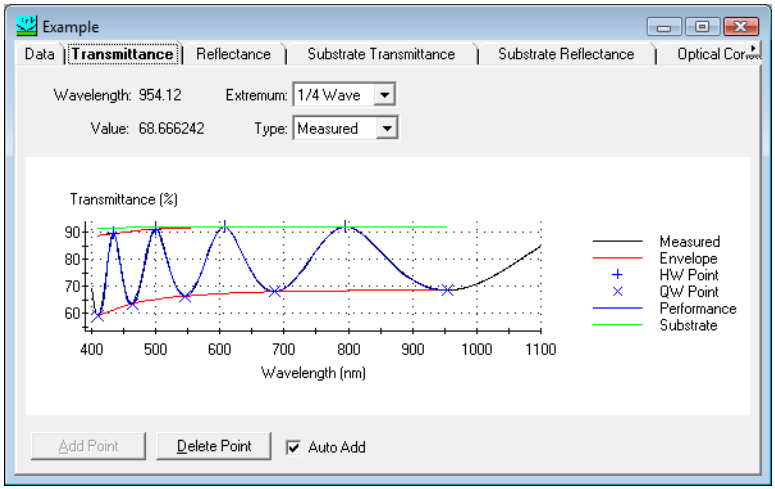
The extraction calculation is launched by selecting **Extract n & k**. There are two stages to the calculation. The first is the interpolation (by cubic spline) of results and the calculation of the refractive index of the substrate. If there is no substrate information, then an advisory message will appear.

The subsequent stage of the calculation actually extracts the optical constants and the thickness of the film. Here the film model becomes necessary. If the figures consist of transmittance only then the film may be assumed to be either homogeneous and absorbing, or inhomogeneous and non-absorbing. If the figures are for reflectance only then the film is assumed inhomogeneous and non-absorbing. If both transmittance and reflectance figures are available then the film is assumed to be both inhomogeneous and absorbing. If an exact match of the measured parameters is found impossible then the measurements are adjusted in accordance with the entered tolerance range and if a good solution is then achieved they will be flagged as **A** for adjusted. If even with permitted adjustment a fit cannot be obtained then results will still be derived but flagged as **B** for bad.

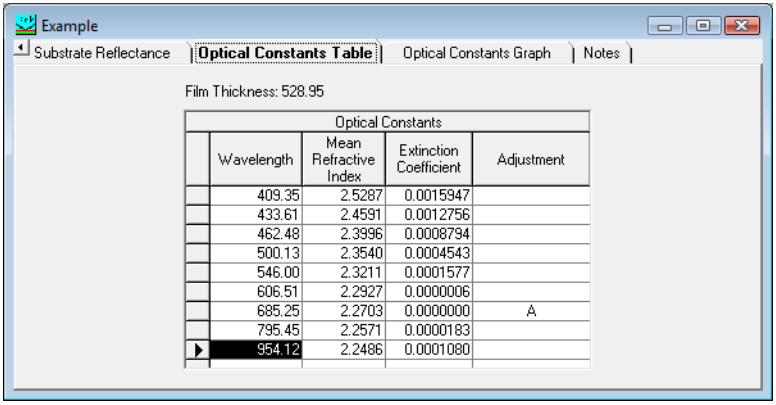
An information box lists any problems. The example below shows some minor problems. The halfwave transmittance points have values slightly greater than the transmittances calculated for an uncoated substrate. Corrections were made within the allowed adjustment zone until the problem disappeared. Calculated results were flagged as "adjusted". Had the corrections eventually exceeded the permitted interval then they would have been flagged as "bad."



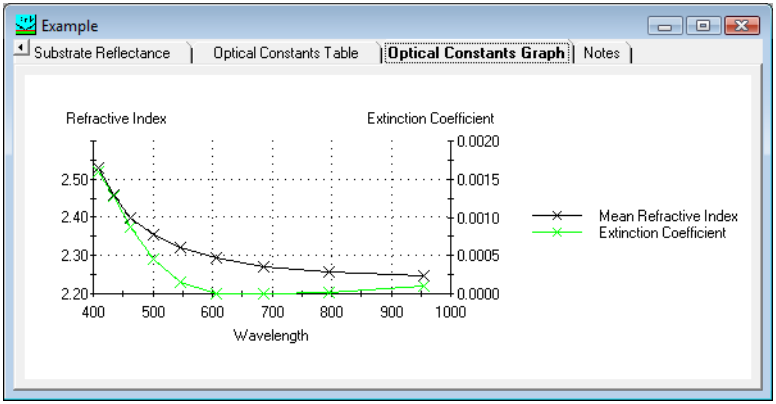
The results of the optical constant extraction are displayed in the form. The transmittance and reflectance tabs will show the calculated performance of the extracted data. This gives a good idea of the validity of the optical constants that have been extracted. These tabs also show the calculated envelopes.



The Optical Constants tab presents a table of the derived optical constants and the derived film thickness.



The data may also be viewed in graphical format on the Optical Constants Graph tab.



Creating materials from the results

Once the calculations have satisfactorily concluded, the material constants must be placed in a material table in the database if they are to be preserved for use. The **Create Material menu** accomplishes this. There are three choices, **From Inner n**, **From Outer n**, and **From Mean n**. If the model used was homogeneous then there will be no difference in these results but they will be distinct if the inhomogeneous model was used.

If examination of the reflectance and/or transmittance curves show that the extrema are not quite matched, we can choose to force the results to match the positions of the extrema rather better by choosing **Match extrema** in the parameters dialog box. This option first calculates the optical constants and layer thickness and then forces the constants to match the extrema.

Matching extrema is most useful when dealing with deterioration in reflectance or transmittance calibration at one end of the scanned range, as, for example, might happen at limit of a given spectrometer. In these cases, the main part of the spectrum is reliable and so the optical constants will be largely correct. The wavelength corresponding to the

outermost extremum is likely to be accurate although the transmittance or reflectance may not be. Then selection of **Match extrema** can very usefully correct the optical constants in the doubtful region without any major effect on those in the reliable zone.

Some precautions

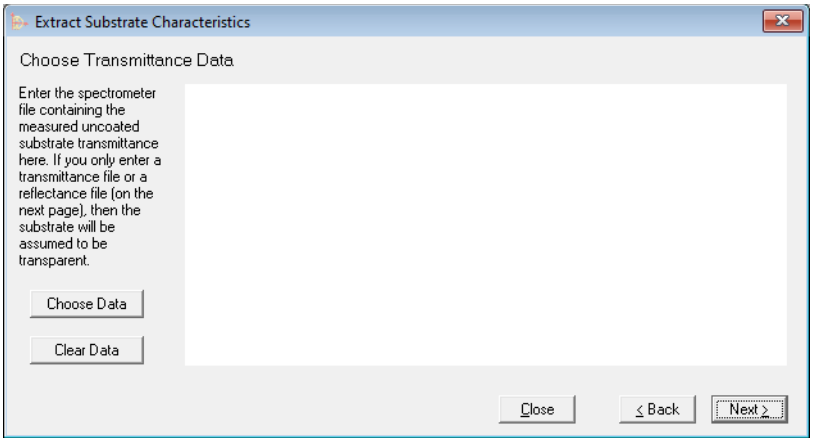
Extraction of optical constants is not an operation like calculating the properties of a design, which has a single, unambiguous result. It involves fitting a model to a set of data and adjusting model parameters until a best fit is obtained. The data are experimental measurements and such measurements will suffer from errors, either systematic or random. The envelope method provided here with the inclusion of the adjustment zones takes care of many of the problems associated with slight data errors but it is still very easy to generate data where no adjustment can possibly achieve a fit. Particularly difficult problems can arise when the coating is almost a perfect antireflection coating for a high-index substrate. Here there are two closely-spaced solutions for the model parameters and there is really no theoretical way of determining which is correct. Under such circumstances the accuracy of a determination can also be very poor. Do remember that any determination of optical constants can be only as reliable as the data from which they are derived. A common and easily recognizable problem is sets of reflectance and transmittance results that add to greater than 100%. A small error, such as that in the data shown above, can readily be accommodated, but such errors can often be substantial. Calibration and maintenance of the instrument on which the measurements are made, is of prime importance.

Obtaining Optical Constants Of A Substrate

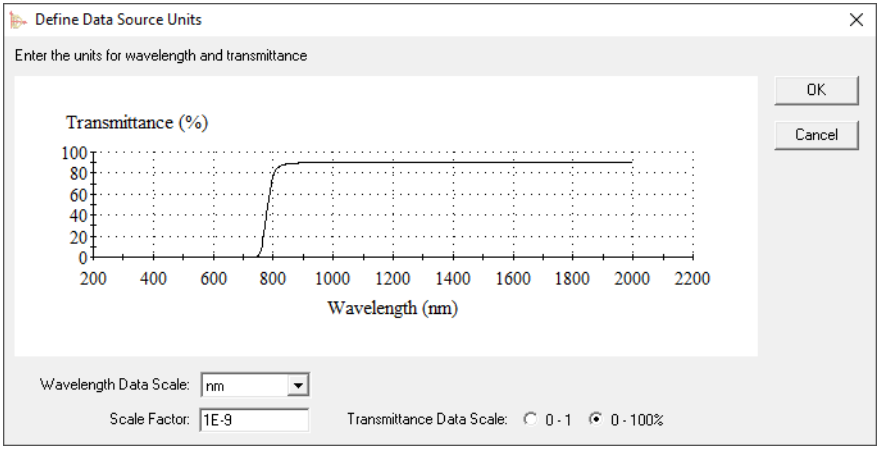
The optical constants of a substrate may be derived from either transmittance and reflectance measurements or reflectance psi and reflectance delta measurements using the **Substrate n,k & T** command in the **Tools** menu. Once the **Substrate n,k & T** command has been selected, the **Extract Substrate Characteristics** window will be displayed. This window is organized as a series of pages that are changed by using the **Back** and **Next** buttons. The **Close** button closes the window.

The first page that is displayed is the **Measurement Type** page. Select between **Spectrometer** and **Ellipsometer** and then click on **Next**. If **Ellipsometer** was selected, the next two pages will be used to enter the Psi and Delta measurements, otherwise Transmittance and/or Reflectance will be entered.

For the Spectrometer case, clicking on **Next** displays the **Choose Transmittance Data** page.



Click on **Choose Data** to select the file containing the transmittance data. After choosing the file, the Import Editor will appear (see the Importing Data section for more information). When the Import Editor has been completed, the units of the data are entered in **Define Data Source** Units.



Select the wavelength units either by choosing a pre-defined unit or by entering a scale factor. Select either 0 – 1 or 0 – 100% for the Transmittance scale. The plot always shows the import data in the current units used by the Essential Macleod. Click on **OK** to continue.

The plot will now be displayed on the **Choose Transmittance Data** page.

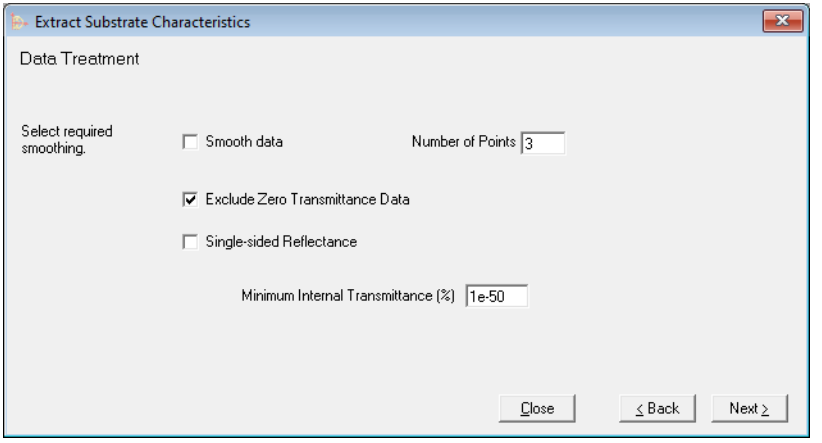
The imported data can be removed by clicking on the **Clear** button. If only reflectance data has been measured, click on **Next** without choosing any data.

Entering Reflectance data is performed in a similar manner.

If only transmittance data or only reflectance data are provided, then the substrate will be assumed to be transparent. That is, its internal transmittance is 100% and the extinction coefficient is zero.

The data files containing the measured transmittance and reflectance data are entered on this page on the Spectrometer tab. Reflectance psi and delta are entered on the Ellipsometer tab.

Clicking the **Next** button on the Choose Reflectance Data page will move you to the **Data Treatment** page. The Data Treatment page allows you to smooth the measured data and to specify other processing options.



Reflectance and Transmittance data may be smoothed by a moving average filter. Checking the **Smooth Data** box causes the data smoothing to be applied to the transmittance and reflectance data respectively. The size of the filter is specified in the **Number of Points** box. For ellipsometer data, Exclude Zero Transmittance Data and Minimum Internal Transmittance are not available. An option to force the extinction coefficient to zero is provided instead.

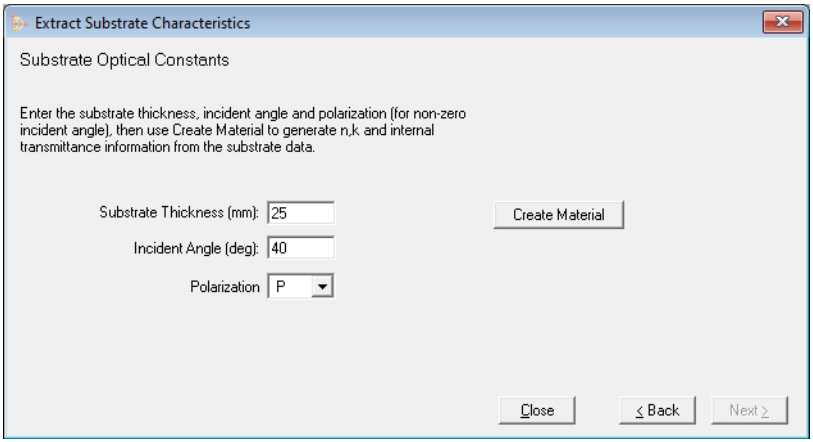
If **Exclude Zero Transmittance** is checked, then any data points with zero transmittance will not be used in the optical constant derivation process.

Check **Single-sided Reflectance** to specify that the second surface reflection was eliminated from the reflectance data. Otherwise it will be assumed that the second surface reflection is included in the reflectance data.

The **Minimum Internal Transmittance** box is used to specify the minimum internal transmittance that will be generated by the optical constant derivation process. If a substrate has no measurable transmittance, then it is not possible to uniquely derive extinction coefficient and refractive index. This option provides an internal transmittance value for use in deriving extinction coefficient and refractive index. Typically if the internal transmittance is set to a very small value (such as 1e-250) this will allow the derivation process to produce a good refractive index derivation. If the Minimum Internal Transmittance is set to zero, the extinction coefficient will be at its maximum value, but

the refractive index values of the non-transmitting region will typically be offset relative to the refractive index values in the transmitting region.

Selecting the **Next** button moves you to the **Substrate Optical Constants** page. Here the thickness of the substrate is specified in the **Substrate Thickness** box. If the measurement was performed at oblique incidence, the **Incident Angle** and **Polarization** can also be specified. Note that all measurements must be performed at the same incident angle and the same polarization. The polarization at oblique incidence must be either s- or p-polarization. For ellipsometer data, the polarization option is not available.



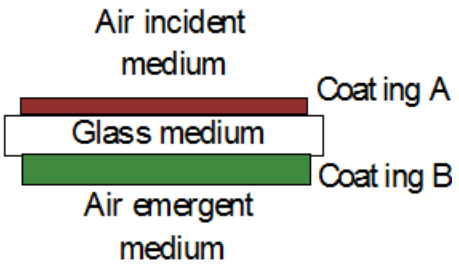
Use the **Create Material** button to create a new material file. This new file can be saved into the current materials database and is then available for use in the program.

STACK

In earlier versions of the Manual, this chapter on Stack was known as Multicoat.

Stack calculates the properties of assemblies of coatings and substrates. The system of elements is known as a **Stack** and it consists of a series of **Media** starting with an **Incident Medium** and ending with an **Emergent Medium**. Each medium, with the exception of the incident medium, may either be uncoated or it may carry one optical coating on its front surface, that is, the surface towards the incident medium. When the only media present are incident and emergent then the system will appear exactly as a single coating on an infinite substrate but usually there will be a number of media with associated coatings.

For example, a system consisting of a single glass plate, with different coatings on either side and incident and emergent media of air, would have incident medium of air, followed by a medium of glass with a prescribed coating on its front surface, followed by an emergent medium of air, also with a coating on its front surface.



Stack3

Stack | Notes

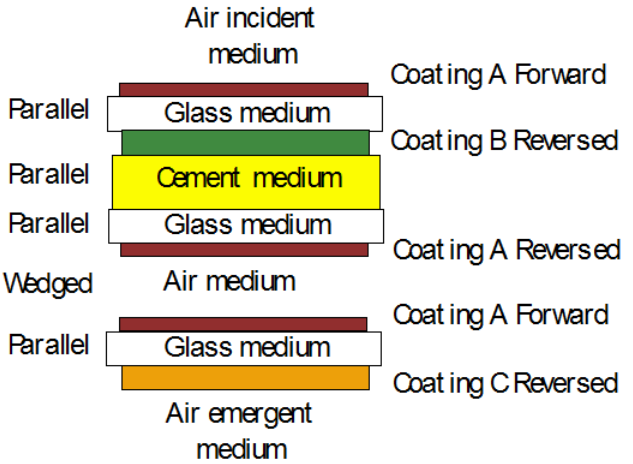
	Medium Type	Medium Material	Medium Thickness (mm)	Coating File	Coating Direction	Coating Locked
	Incident	Air				
	Parallel	Glass	1.000	a	Forward	No
▶	Emergent	Air		b	Reversed	No

Note that the coatings are defined by reference to the appropriate design files. In design file b.dds the order of the layers runs from an incident medium of Air to a substrate of Glass but in the stack it is being used in the opposite direction with its substrate defined as Air and its incident medium as Glass. The coating direction is therefore labeled as **Reversed**. Coating a.dds, on the other hand has the label **Forward.**

Media are specified by their optical constants and internal transmittance. The interfaces, or boundaries, of the media are assumed either to be sufficiently parallel so that all the reflected beams remain within the aperture of the system or sufficiently wedged so that the reflected beams are directed outside the system aperture.

Nevertheless, in either arrangement, the aperture of the system is such that normal incidence in the incident medium implies normal incidence throughout the stack.

The next figure shows an arrangement of a more complicated stack. Here there are seven media and five coatings. The air medium is thought to be sufficiently wide to avoid problems of multiple reflections and so it is labeled as Wedged. The other media are labeled as Parallel because multiple beam effects do occur. The Stack window shows the structure of this more complicated stack.



Stack3

Stack | Notes

	Medium Type	Medium Material	Medium Thickness (mm)	Coating File	Coating Direction	Coating Locked
	Incident	Air				
	Parallel	Glass	2.000	a	Forward	No
	Parallel	Cement	0.100	b	Reversed	No
	Parallel	Glass	2.000	None		
	Parallel	Air	25.000	a	Reversed	No
	Parallel	Glass	1.000	a	Forward	No
▶	Emergent	Air		c	Reversed	No

In all cases, designs of coatings are already established and the specification of the stack simply lists the names of the files in which these designs are already stored. The coatings are given the attribute **Coating Direction** that can be either **Forward** or **Reversed**. The arrangement in the coating file assumes an order for the layers from incident medium through to emergent medium. In a stack, however, the orientation may be such that the support (i.e. substrate) for the coating may turn out actually to be the incident medium. In other words, the coating may be pointing in the opposite direction. Such an orientation is known as **Reversed**. The normal orientation is known as **Forward**.

These attributes are assigned automatically in the first instance and the designations will usually be correct. However a click in the appropriate box will toggle the designation should the automatic assignment need to be changed.

The media have the attribute **Medium Type** and this can be **Incident**, **Emergent**, **Parallel** or **Wedged**. **Incident** and **Emergent** are automatically assigned to the first and last media respectively in the stack and these attributes cannot be changed. All other media must be either **Parallel** or **Wedged**. **Parallel** implies that all the beams reflected backwards and forwards in the medium are within the aperture of the system and so are incoherently combined. **Wedged** implies that the surfaces of the medium depart sufficiently from parallelism that the reflected beams within the medium are directed out of the aperture of the system. Since the incident medium and emergent medium are semi-infinite they are neither parallel nor wedged. As with **Coating Direction**, a click in the appropriate box toggles the designation.

The material files contain refractive index and extinction coefficient information and should, theoretically, be capable of yielding an estimate of transmittance once the thickness of the medium is defined. However, extinction coefficient is not a useful way of specifying transmittance of a massive medium. Internal transmittance is much more reliable. Internal transmittance is the transmittance that exists between the inside of the front surface and the inside of the rear surface, that is the part of transmittance that relates to the medium but excludes reflection losses at the interfaces. A Material, therefore, may also include an internal transmittance definition. The internal transmittance can be specified as Lossless, i.e. 100% transmittance for all wavelengths, or as a table of values. For cases where the extinction coefficient data is better than no data, the internal transmittance can be calculated from the extinction coefficient. Media are specified by a Material and a thickness. Since the internal transmittance figures relate to one particular thickness of material then the actual thickness of material in the stack must also be specified. See Internal Transmittance in the Materials Management chapter for more information concerning Material documents.

Internal transmittance

The losses in a thick plate with flat surfaces are due to a combination of absorption and reflection. If we can remove the reflection losses by application of perfect antireflection coatings then the resulting transmittance of the plate is the quantity known as internal transmittance. The internal transmittance of a completely homogeneous plate is related to both absorption coefficient and extinction coefficient and, strictly, can be calculated from either. Why when we already have extinction coefficient tabulated for our materials do we introduce internal transmittance? The reason is that extinction coefficient is not a good parameter for the characterization of relatively thick slices of material. Imagine an extinction coefficient at 1000nm of 10^{-5}. In terms of thin films, this is extremely small and very difficult to measure with any degree of accuracy. The relationship between extinction coefficient and absorption coefficient is

$$\alpha = \frac{4\pi k}{\lambda}$$

where the units of absorption coefficient, α, will be the inverse of those of wavelength, λ. Our extinction coefficient gives an absorption coefficient of 1.26cm^{-1} and an internal transmittance of a 1cm thick plate of 28.4%. A change in extinction coefficient to 2×10^{-5}, still very small in thin film terms, changes the transmittance of the plate to 8%. If we are calculating the transmittance of a slice of material rather than a thin film either internal transmittance or absorption coefficient is a more suitable quantity than extinction coefficient. One other point is that extinction coefficient is sometimes measured from the surface properties, for example by ellipsometer. Under those circumstances surface effects that hardly change the transmittance of the component can have a large effect on measured extinction coefficient, which is then a quite misleading quantity to use for bulk transmittance calculations.

Thick media in a Stack or Design, therefore, use internal transmittance as the definitive parameter for assessing the transmittance of a medium. This is chosen over absorption coefficient, equally suitable, because frequently material data are supplied in that form, especially colored filter glasses.

The conversion from absorption coefficient to internal transmittance in percent is

$$T_i = 100\exp(-\alpha d)$$

where *d* must be expressed in the same units of length as α, and is to be entered into the substrate file. Usually 1mm is the standard thickness for the files while α will be in cm-1 and so the value to be entered will be 0.1cm. The tables will usually have units of mm and so the value to be entered in the tables will then be 1mm.

Sometimes the extinction coefficient in published tables has been derived from measurements of transmittance of thick samples. In that case the extinction coefficient may then be used to derive internal transmittance. We will see later that an optional alternative for data entry into the internal transmittance tables is internal density. If wavelength is given in nm and the standard thickness for the table is 1mm then the conversion from extinction coefficient to internal density is

$$D_i = 5.4575\times10^6\frac{k}{\lambda}$$

Do make sure, if you are using this expression, that the values are entered into the tables as density and not transmittance.

Transmittance and Density

Can a transmittance of zero actually exist? Light is attenuated on traversal of a medium by a number of processes. It is absorbed and it is scattered and there may even be generation of light with either the same or a changed wavelength. Light of wavelength 1000nm with an irradiance of 1Wm^{-2} has a photon flux of 43.5×10^{22} photons per square metre per day. A transmittance of 2.3×10^{-24}, that is a density of 24.36, will reduce this flux to one photon per square metre per day. A further reduction by a factor of 365, that is a density increase to 26.2, will reduce the flux to one photon per year and a further increase of 2.0 in density to one photon per century.

Clearly a density of 30 or so is not something that is susceptible to direct measurement at the present time and in practical terms anything that is greater than that in density is for all practical purposes equivalent to zero transmittance.

Internal transmittance is the definitive parameter rather than density because it is usually the published parameter and because most often it is the overall transmittance of the system that is most important. However there is the problem of how to convert an internal transmittance of zero into a value of density. Strictly speaking this should be a density of infinity but can we really tell the difference between a transmittance of 0.000000000000000000000001% and 0.00000000000000000000000001%? We certainly cannot measure them, and both will tend to be shown as zero in the tables of results, unless the formatting has been changed from the default, but the corresponding densities will differ by unity. There is no completely satisfactory way of handling the problem of low transmittances and high densities. In the Essential Macleod the convention is that the greatest density is 40. Zero transmittance is therefore interpreted as a density of 40. In the above example this corresponds to one photon every 10^{14} years or so.

For overall transmittances corresponding to densities of less than 40, then, the results are considered to represent genuine transmittance. When the density becomes greater than around 40, the transmittance is set to zero and the corresponding density to 40. This applies equally to stacks or to internal transmittance data.

This may occasionally cause a problem when internal transmittance data correspond to much greater thicknesses than are used in a particular stack. Since the internal transmittance is the definitive value it will be interpreted as zero and the density will remain at 40 whatever the thickness.

A related problem can occur when dealing with very high transmittances in extremely thick media when the internal transmittance data refer to much thinner samples.

Caution should be used therefore when thicknesses of substrate or media material in a stack are either much less or much greater than in the material tables. It may be necessary to set up a new material file where the thickness is much nearer the actual thickness used in the calculations.

Refinement and Synthesis

Refinement options are described in detail in the Refinement and Synthesis chapter of this manual. For refinement in a stack, however, there are some additional conventions that are described here.

The refinement menu is found under **Parameters**. **Tools** exist for entering targets, adjusting refinement parameters and performing refinement. These menus are similar to those provided for refinement of single coatings. The **Coating Locked** column in the stack window specifies that a particular coating in the stack will not take part in the refinement. Only coatings with a **Coating Locked** value of **No** will take part in refinement.

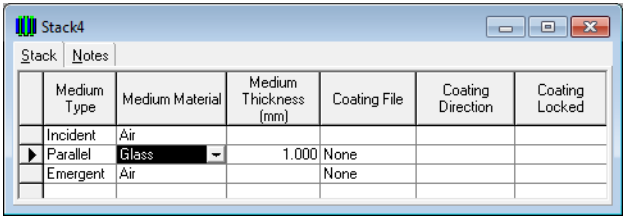
Coatings are implicitly linked by name in a stack. If the same coating design file is used on more than one surface in a stack, then refinement will adjust a single copy of the design and apply it to all surfaces using the same design name. If you want to allow refinement to treat all coating designs separately, but want to have the same starting

point, then the design must be copied to new files, one for each surface that is to have the same starting point.

Stack Menu

This menu is obtained when the Stack window is active. We illustrate its use with an example.

If in the **New...** dialog box from the **File** menu we select **Stack** and click **OK** it brings up a new Stack window. It may be necessary to drag the right-hand boundary to reveal all of the columns.

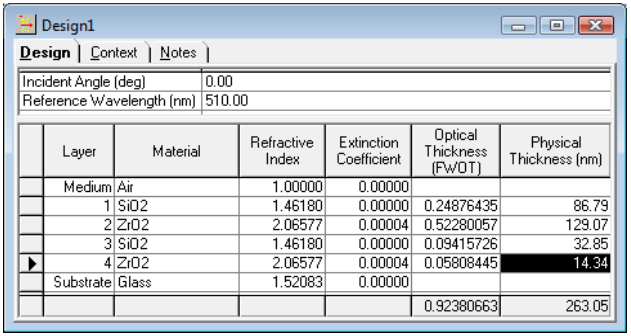


	Medium Type	Medium Material	Medium Thickness (mm)	Coating File	Coating Direction	Coating Locked
	Incident	Air				
▶	Parallel	Glass	1.000	None		
	Emergent	Air		None		

The first three columns apply to the media of the stack. The final three columns are concerned with the coatings. Since this is a new stack it is very simple and consists of an incident medium of air, a parallel-sided medium of glass and an emergent medium of air. There are no coatings.

We will now calculate the properties of a parallel-sided glass substrate with an antireflection coating on each side.

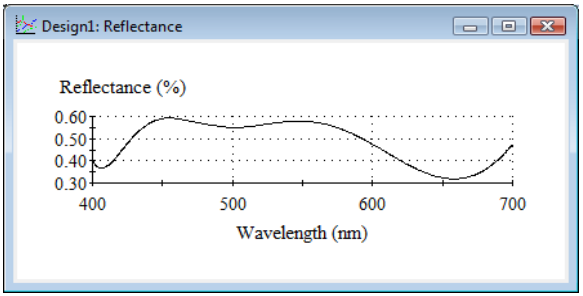
First we need to create the antireflection coating. We can do this by selecting **New** from the File menu again and creating a design that is shown in the next figure. Note that because this is a multiple document interface, it is unnecessary to close the stack window. It can remain open.



Incident Angle (deg)	0.00
Reference Wavelength (nm)	510.00

	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
	Medium	Air	1.00000	0.00000		
	1	SiO2	1.46180	0.00000	0.24876435	86.79
	2	ZrO2	2.06577	0.00004	0.52280057	129.07
	3	SiO2	1.46180	0.00000	0.09415726	32.85
▶	4	ZrO2	2.06577	0.00004	0.05808445	14.34
	Substrate	Glass	1.52083	0.00000		
					0.92380663	263.05

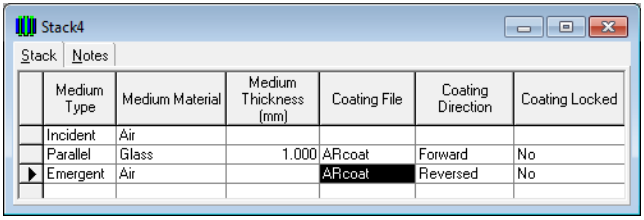
This is an antireflection coating with performance shown in the next figure.



Now we will save this design and we can conveniently choose the name ARcoat.DDS.

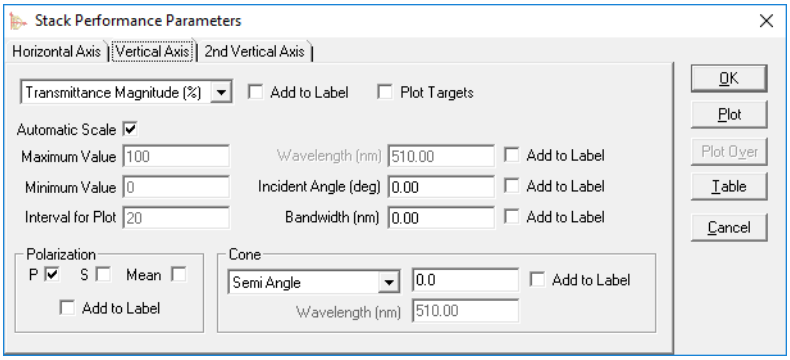
If we return to the stack window, by clicking in it or by selecting it from the **Window** menu, we can now complete the new stack. We simply have to add the two coatings. We double-click on the Coating File cells in the second and third rows and select the file ARcoat.dds. The directions given in the next column should automatically be assigned but if they are not as in the figure then they should be changed by clicking in them to toggle them.

This describes a stack consisting of incident and emergent media of air surrounding a glass disk with parallel sides that has an antireflection coating given by design file ARcoat.dds on either side. The convention in adding coating files to the stack window is that the medium on the same row as the coating is taken to be its emergent medium. Row 2, for example, shows a coating with emergent medium glass and incident medium, from the row above, air. This is the normal configuration for an antireflection coating design file and so the **Coating Direction** is listed as **Forward**. In row 3 the emergent medium is air while the incident medium, from the row above, is glass. This means that the **Coating Direction** should be set as **Reversed**.



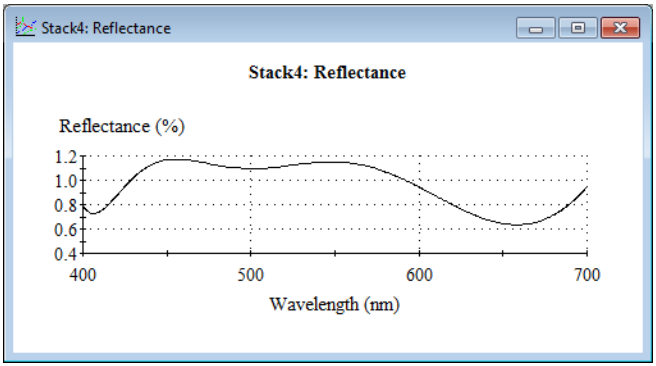
	Medium Type	Medium Material	Medium Thickness (mm)	Coating File	Coating Direction	Coating Locked
	Incident	Air				
	Parallel	Glass	1.000	ARcoat	Forward	No
▶	Emergent	Air		ARcoat	Reversed	No

Now we set the performance parameters by selecting **Performance...** from the **Parameters** menu.



The **Stack Performance Parameters** dialog box is similar to others in the package. Like the corresponding menu for a design with a thick medium, it includes cone and bandwidth calculations. See the Coherence, Cone, and Bandwidth section of the Essential Macleod Structure chapter for more information. Once the parameters are considered satisfactory, the plot and/or table can be calculated. Selecting **Plot** in the **Performance** menu gives the following graph. This is the reflectance of the glass disk with antireflection coating on both sides.

The stack and its performance can be saved in the normal way.



Now let us set up a more complicated stack consisting of two glass substrates arranged in series, one coated on either side with the antireflection coating we have been using and the other with only one side coated. Air is the incident and emergent medium and there is air in between the two substrates. The surfaces of the substrates are parallel but the space in between is wedged.

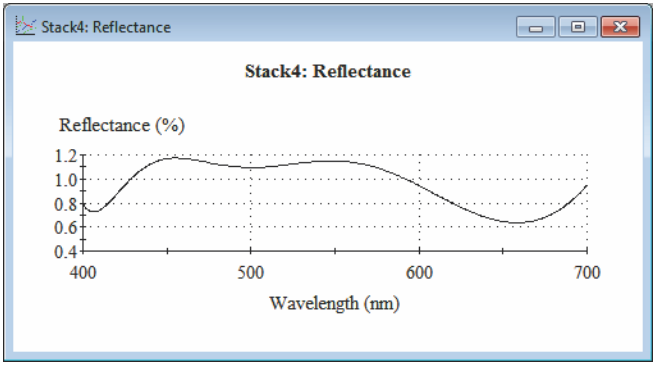
To do this we load the existing stack and save it as Trial2, say. Then we insert two additional media. The new stack is shown in the following window. Note that it may be necessary to remove a coating. To do this, select the appropriate cell and press **<Del>**. The entry will change to **None**. To alter **Parallel** to **Wedged**, or vice versa, click in the appropriate cell to select it and then click once to change it.

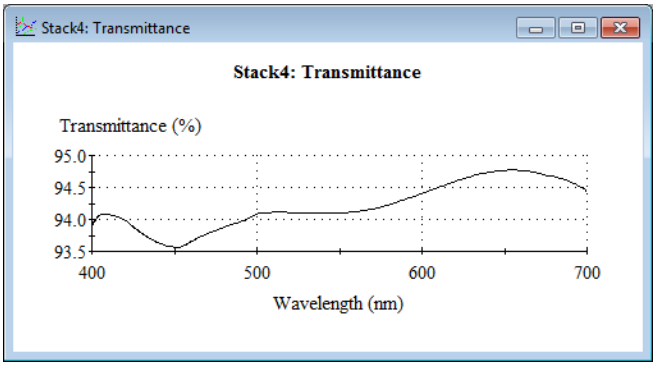
Stack4

Stack | Notes

	Medium Type	Medium Material	Medium Thickness (mm)	Coating File	Coating Direction	Coating Locked
▶	Incident	Air				
	Parallel	Glass	1.000	ARcoat	Forward	No
	Wedged	Air	1.000	ARcoat	Reversed	No
	Parallel	Glass	1.000	None		
	Emergent	Air		ARcoat	Reversed	No

The reflectance and the transmittance both as functions of wavelength are shown below. The reflectance curve shows almost no reflectance but the transmittance curve shows a loss of over 4% in transmission. This is because of the wedging of the space between the two substrates. This means that light reflected from the surface of the second component does not enter the aperture of the receiver and is therefore lost. The reflected light is from the first component and since that is efficiently antireflected, little is received and the reflectance is low. The light reflected from the second component, one surface of which is uncoated, is lost to the transmitted beam and so the transmittance of the overall system is reduced. In the blue region it is reduced a little further by absorption in the coatings. Experimenting in this way with wedged and parallel surfaces can help in assessing the amount of stray light or veiling glare in transmitting optical systems. If the components of an image forming system are all set as wedged, then this will be the transmittance of the image-forming light. If now the components are all set to parallel and the transmittance reassessed, it will be found to be higher. The increase is due to potential stray light. In this particular example, even with one surface untreated, the potential stray light is quite small.




Stack4: Transmittance
Stack4: Transmittance
Transmittance (%)
95.0
94.5
94.0
93.5
400
500
600
700
Wavelength (nm)

ANALYSIS AND DESIGN TOOLS

The tools that are classified under Analysis and Design permit calculations beyond straightforward performance and provide aids in the design of certain specific types of coating. Analysis facilities that help in understanding designs are admittance diagrams, amplitude reflection loci and electric field distribution. Design tools include nonpolarizing edge filter design, potential transmittance calculations and induced transmission filter design as well as Herpin equivalents.

The materials used in the Essential Macleod are dispersive. The calculations carried out by the Analysis enhancement are almost all with respect to a particular wavelength.

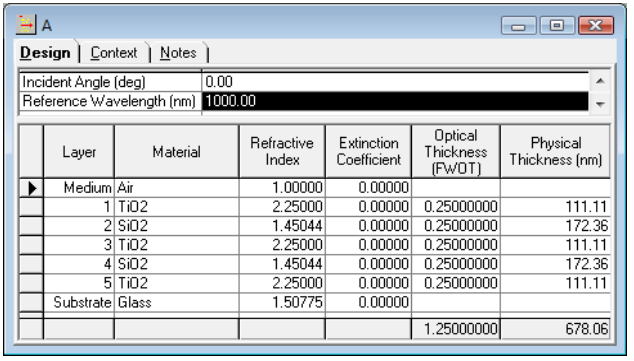
To gain access to the Analysis and Design tools, a design window must be active. Then the Tools menu provides the route to the Analysis and Design tools.

The Analysis tools are not available when there are thick layers in the design.

Analysis Submenu (Design)

The **Analysis** submenu has six options. **Admittance...**, **Reflection Coefficient...**, **Electric Field...**, **Absorptance Rate...**, **Total Absorptance...**, and **Performance Envelope…**. These differ from the options in the Essential menu in that they concentrate on internal properties of the coatings rather than overall performance. Thus, they are collectively referred to as **Analysis**.

We deal with each in turn but the details are broadly similar. Selection of the menu item brings up a dialog box for modification of the various calculation parameters including wavelength, or acceptance of the defaults. This dialog box also includes buttons that launch generation of plots or tables. The design used to generate the following plots is a simple five-layer quarterwave stack.



	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
▶	Medium	Air	1.00000	0.00000		
	1	TiO2	2.25000	0.00000	0.25000000	111.11
	2	SiO2	1.45044	0.00000	0.25000000	172.36
	3	TiO2	2.25000	0.00000	0.25000000	111.11
	4	SiO2	1.45044	0.00000	0.25000000	172.36
	5	TiO2	2.25000	0.00000	0.25000000	111.11
	Substrate	Glass	1.50775	0.00000		
					1.25000000	678.06

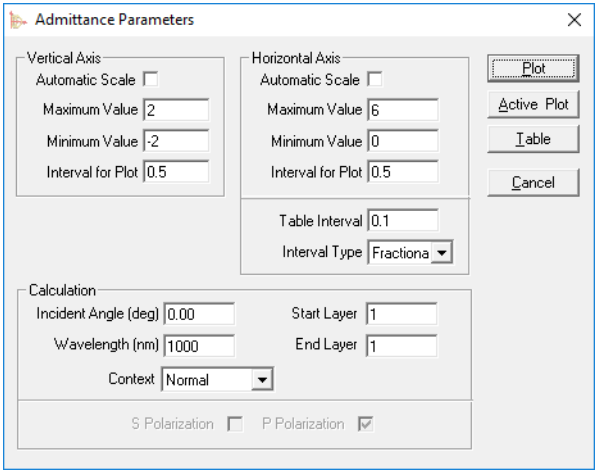
Plot and Plot Over

Note that in all cases the plotting in Analysis is initiated by the **Plot** button in the **Parameters** dialog box rather than as a menu item. The **Plot Over** menu command is not available in Analysis. To plot a second curve over a first, therefore, the second plot should be created on its own in the normal way and then dragged onto the first plot.

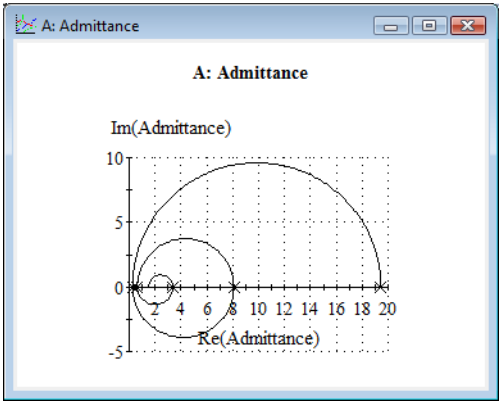
Active Plots are also available for Analysis functions (except Total Absorptance) by clicking the **Active Plot** button.

Admittance...

Selection of this menu item begins the calculation of the variation of optical admittance through the coating. In graphical form the results form an admittance locus in the complex plane. First a dialog box appears that carries the various parameters that must be specified for the calculation.



Vertical axis and horizontal axis cover the two coordinate axes. The horizontal scale factor is normally fixed equal to the vertical so that circular loci appear truly circular. This means that the vertical and horizontal extents of the plot are not independent. However this can be changed as detailed below. The Table interval is simply the thickness interval between points in the admittance table. However this interval can be either fractional or absolute. Fractional means that each thickness increment is the thickness of the appropriate layer times the stated interval. Absolute means that the thickness increment will be equal to the stated interval. A constant fraction of layer thickness is useful when some layers are very thick and considerable time could be wasted in unnecessarily detailed calculations of their properties or when some layers are very thin and would receive almost no calculation points at all. To avoid awkward numbers, the fractional increment is rounded down to the nearest convenient number. Incident angle and wavelength are also to be specified. If the angle of incidence is other than zero then the polarization may be specified. The full admittance diagram of a complicated coating is sometimes virtually impossible to follow because of the way in which the loci lie over each other. Thus it is possible to select a restricted range of layers for plotting. This restricted range does not change the locus of any layer. It is simply that the layers outside the range do not have their loci plotted although they still take part in the calculation.

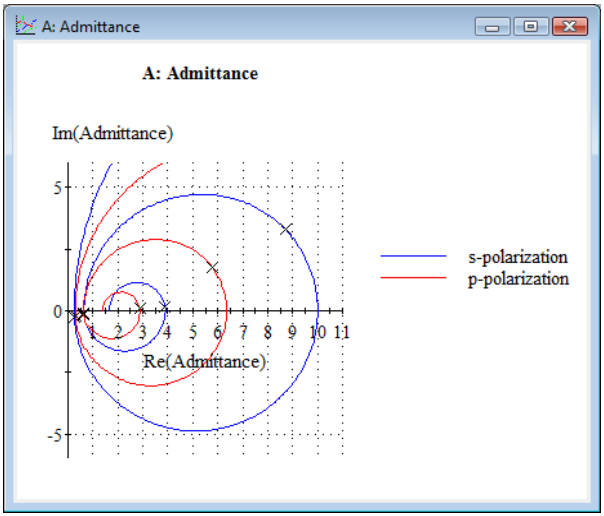


In the tables, admittances are always calculated at the interfaces between layers even if they do not correspond exactly to the thickness increments. Reflectance and phase changes on reflection are also calculated with the assumption that the incident medium is that specified for the coating.

A feature of the program is that negative thickness increments can be entered in the tables. (Note that this does not apply to the plots.) The admittance variation will then be calculated as though the layers had negative thickness. This technique is useful for the design of systems where there are heavily absorbing layers. If the design is set up with the order of layers reversed and the substrate with an admittance equivalent to the desired admittance for the coating then a negative increment will draw the admittance diagram backwards. This shows the feasibility of the attempted performance. If, for example, the locus wanders into the second or third quadrant of the complex plane then the desired performance is completely impossible without some substantial changes.

Note that at oblique incidence it is the modified admittances that are plotted. The modified admittances are the result of a normalization of the admittances so that the incident medium remains constant in spite of either the tilts or the plane of polarization. The use of modified admittances makes the interpretation of the diagram much easier. Plots at oblique incidence have full lines for s-polarization and broken lines for p-polarization throughout the package although these can be altered in any plot by the line editor. To activate the line editor the mouse should be double-clicked with the cursor inside the plot area. The line that will be edited is that nearest to the cursor.

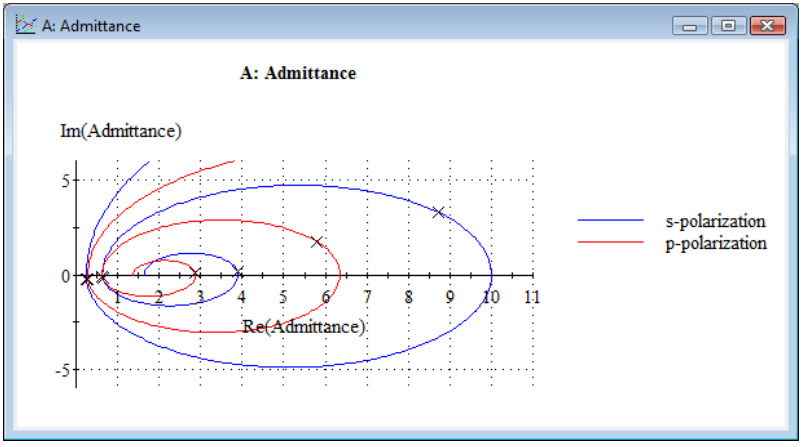
A typical plot of the admittance diagram at 30° angle of incidence is shown below. Both s- and p-polarizations have been drawn with thicker lines (s-polarization is blue and p- is red in the original). The ends of the loci are somewhere off the top of the diagram.



To resize the plot and allow the loci terminations to be seen the vertical axis can be changed. Recalculation is unnecessary.

With the plot as the active window select **Edit** and then **Parameters...**. The **Plot Parameters** dialog box will appear. The vertical scale can then be changed in range to -6 to 15 (with appropriate change to the interval also). The result is shown below. The horizontal axis has shrunk accordingly, although the terminations can now be seen.

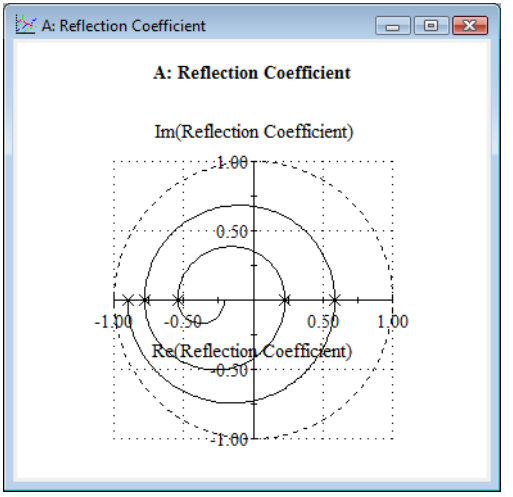
It may be more useful to permit the plot to expand to use up the wide space to the right of the window but simply altering the horizontal scale is not useful because the admittance locus will not change. An alternative is simply to uncheck the box labeled **1 to 1 Aspect Ratio** in the **General** area of the **Plot Parameters** dialog box. This gives the result shown in the next figure. Whether or not this will be useful depends on personal preference but the facility is there should it be wanted.



Admittance loci in structures like quarterwave stacks can vary rapidly from very small to very large loops. In extreme cases this can cause problems in plotting because the outer right hand part of the loop will be executed at enormous speed compared with the left hand part. The adaptive plotting of the package will normally accommodate this but there can be cases where even the adaptive plotting is overcome and it is clear to the user that a loop has collapsed. If this happens then the **Nominal Plot Segment Length** in the **Essential Macleod Options** box, activated by **General...** in the **Options** menu, must be reduced. This is usually set at 0.01, adequate for virtually all cases. If it must be changed then the change should be small. 0.001 will usually be as small as ever required. Be careful with alterations. A small value means more points and a reduction by a factor of ten means ten times as many points in the plot taking ten times as long and ten times the storage. Make sure to change the value back to the default of 0.01 immediately it is no longer required otherwise all plotting will suddenly become very slow.

Reflection Coefficient...

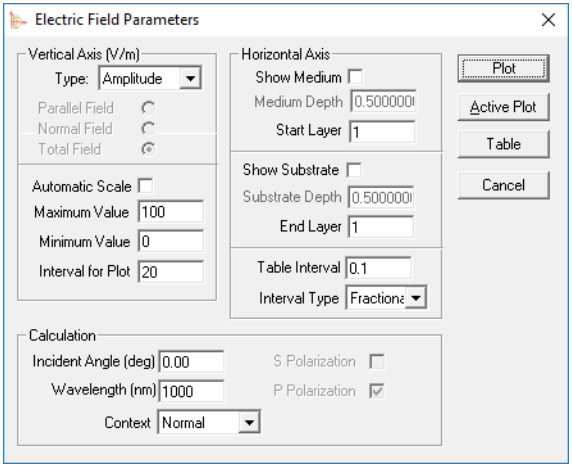
The variation of complex amplitude reflection coefficient, with incident medium for the reflection coefficient calculation always equal to the incident medium for the coating, gives a locus in the complex plane that is similar in some respects to an admittance locus. The variation of reflection coefficient for a dielectric film is circular, just like admittance. As with the admittance loci, the **Plot Parameters** dialog box permits uncoupling of the scale factors of horizontal and vertical axes should this be required.



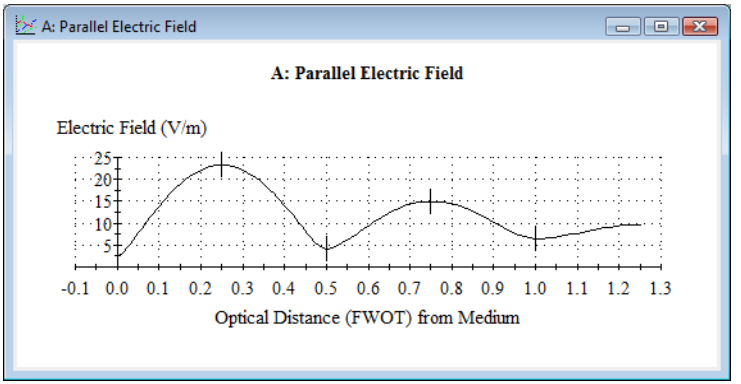
Electric Field...

The performance of a thin film coating depends on interference effects and the interference results in standing waves. The variation of electric field amplitude accompanying these standing waves can be considerable. Losses due to absorption and scattering are highest where the electric field is highest and so the distribution of electric field is an important tool in the design and/or analysis of coatings where either losses are to be very low or very high. A particular feature of **Electric Field...** is that absolute amplitude values are calculated. Calculations of field through multilayers are frequently

normalized to the value at a given interface, principally because so much normalization exists in normal calculations that it is difficult to keep track of it. It is not always easy, particularly at oblique incidence, to relate these normalized fields to known incident irradiances. Here an incident irradiance of 1 watt per square metre measured using a detector placed normal to the beam direction is assumed and the electric field amplitude is given in volts per metre throughout the multilayer for either s- or p-polarized light. For s-polarization the fields are all parallel to the interfaces but for p-polarization there are components which are normal to the interfaces. There is not necessarily a simple phase relationship between these components and so a calculation of total field is included. The **Electric Field Parameters** dialog box includes the choice of Parallel, Normal or Total Field. The Electric Field Intensity can also be calculated and this is defined as the square of the electric field amplitude divided by the square of the normal input field amplitude in Air which for an incident irradiance of 1 watt per square metre is approximately $(27\ V/m)^2$



The **Electric Field Parameters** dialog box is similar to all the others but there are two choices that should be further explained. There are two check boxes **Show Medium** and **Show Substrate** in the Horizontal Axis section. The standing wave pattern exists also in the incident medium. Although there is no standing wave in the substrate, if there is absorption or if the calculation is beyond the critical angle then there will be an exponential decay. Both these can be shown by ticking the appropriate box. When the box is ticked then the depth into either substrate or incident medium can be specified. Usually the default value of 0.5 will be adequate. This value is in terms of full waves at the reference wavelength. Once the **Show Medium** and/or **Show Substrate** boxes have been checked it becomes impossible to select a limited range of layers for display. The plots of electric field assume incident light coming from the left (as is normal) so that the substrate is over on the right.

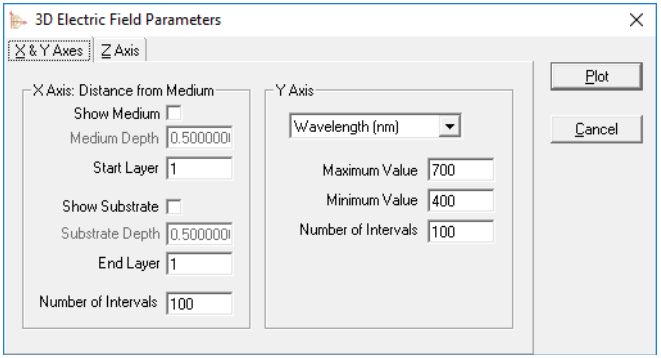


3D Electric Field...

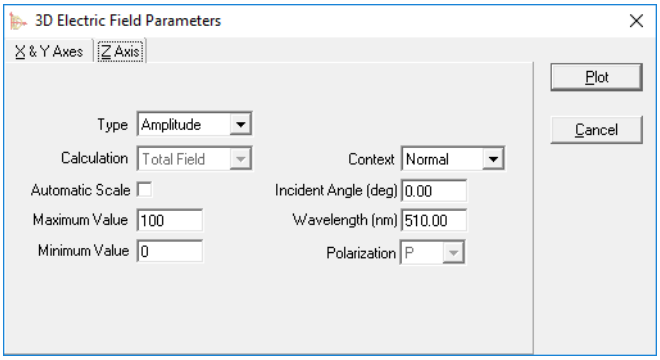
The 3D Electric Field command extends the Electric Field command so that electric field is plotted as a function of a second parameter that is either wavelength or incident angle as well as the position in the coating.

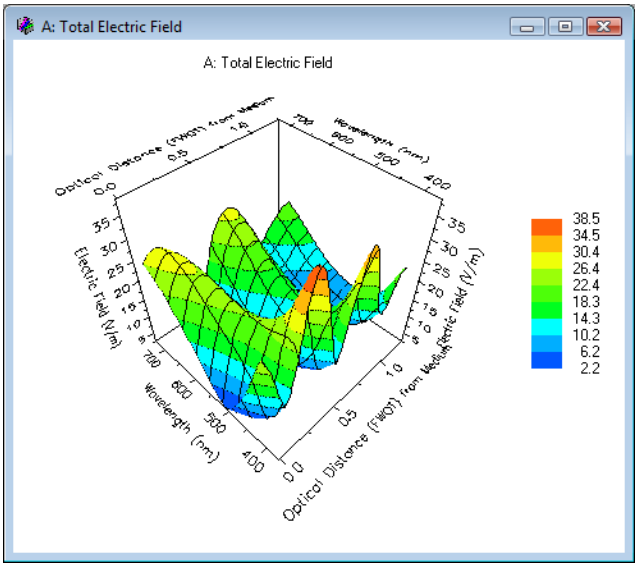
The X axis parameters provide the same control over which part of the deisgn is used for the calculation. Table Interval and Interval type are not included because the 3D version does not produce a data table. Instead, Number of Intervals is used to specify the total number of points calculated in the X direction. These points are equally spaced across the range of X values.

The Y axis is used to specify the parameter used and the value range. Either wavelength or incident angle may be specified. Maximum and minimum values are also specified. Number of Intervals specifies the total number of points calculated in the Y direction. These points are equally spaced across the range of Y values.



On the Z axis, Incident Angle is only used when the Y axis parameter is Wavelength and Wavelength is only used when the Y Axis Parameter is Incident Angle.

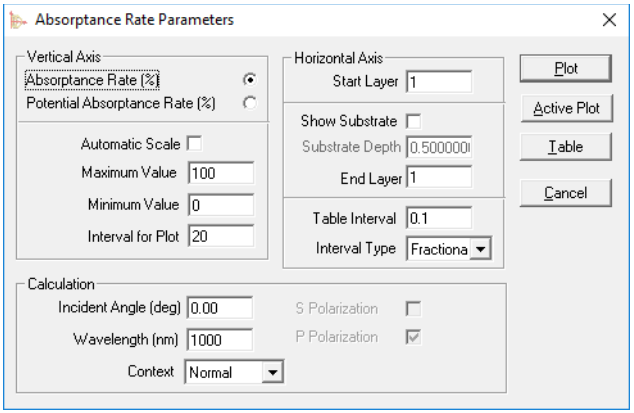




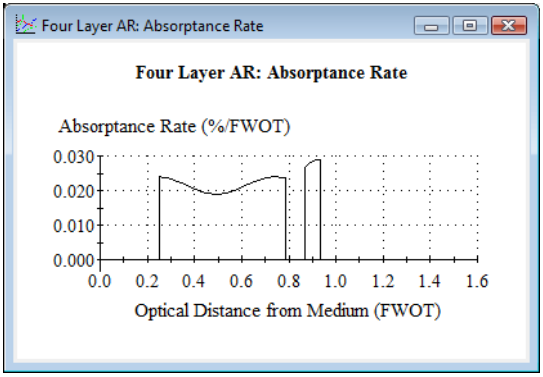
Absorptance Rate...

This starts the calculation of the Absorptance Rate of the coating. The absorptance rate is given in terms of % Absorptance per unit thickness in the current thickness units. Either the absorptance rate or the potential absorptance rate may be plotted. The table always shows both absorptance rate and potential absorptance rate. The potential absorptance rate is the maximum absorptance rate of the coating if all incident energy were either transmitted or absorbed.

Before the results are presented, a dialog box is displayed in which the various parameters for the calculation are specified.



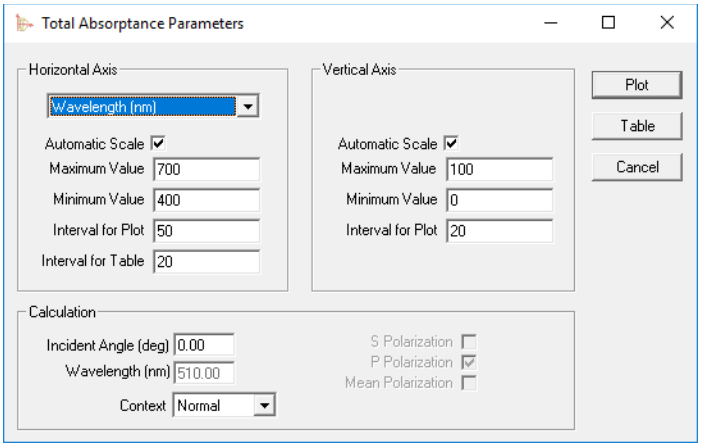
The **Absorptance Rate Parameters** dialog box is similar to the other Analysis dialog boxes. The **Vertical Axis** options allow you to choose between **Absorptance Rate** and **Potential Absorptance Rate** for the plotted curve (tables always show both Absorptance Rate and Potential Absorptance Rate). The **Horizontal Axis** allows you restrict the range of layers for which absorptance rate calculations are performed, or you can show absorptance rate in the substrate if desired. The **Substrate Depth** field allows you to specify the distance into the substrate for which absorptance rate calculations will be performed in the current thickness units.



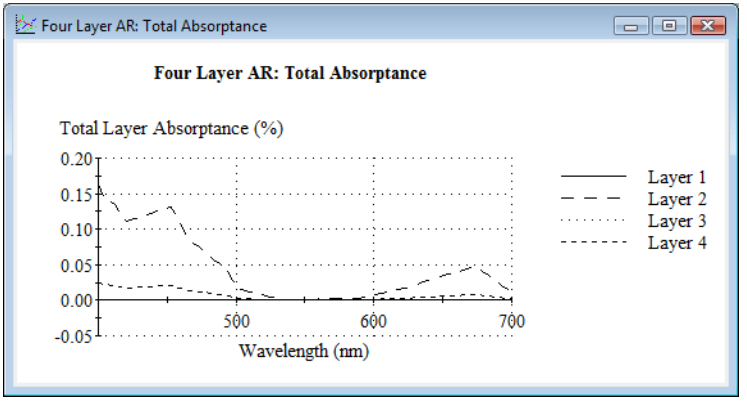
The plot shows the absorptance rate for an initial antireflection coating design where two of the layers have some absorption and the other three do not.

Total Absorptance...

The Total Absorptance calculation shows how the absorption of the whole coating is split amongst the individual layers of the coating. A dialog box is displayed before the calculations are performed so that you may enter desired parameters for the calculation.



You can specify a wavelength, frequency or incident angle range for the horizontal axis. Where a wavelength or frequency range has been specified, the total absorption will be calculated at the Incident Angle in the Calculation box. Where an incident angle range has been specified, the total absorption will be calculated at the Wavelength in the Calculation box. If there are no selected layers in the design, then the total absorptance will be calculated for all layers in the Design. If one or more layers are selected, then the total absorptance will only be calculated for the selected layers.



The plot shows the total absorptance of each layer of an initial anti-reflection coating design. Layers 1 and 3 have no absorptance, but layers 2 and 4 have a small amount of absorptance.

Performance Envelope...

For a selected layer in the design, **Performance Envelope** calculates the maximum and minimum possible transmittance over all values of thickness of the layer. It also calculates the round-trip phase change in the layer. When the round-trip phase change is in the immediate vicinity of 0 or $2m\pi$, where m is an integer, the coating performance

will match the maximum envelope. When the gap between the maximum and minimum envelopes is large, the performance will tend to be close to the minimum except when the 0 or $2m\pi$ condition is very closely satisfied.

The performance envelope is very useful for assessing the sensitivity of a design to errors in the thickness of the selected layer. Since the performance envelope marks the limit of performance whatever the variation in thickness of the selected layer, it represents the limit of performance for any possible thickness error, no matter how large, in the layer. The crossing points of the round-trip phase change curve with the zero phase axis mark those points where the actual performance curve will touch the maximum envelope. The slope of the round-trip phase curve at the axis crossing indicates the sensitivity of that particular feature to layer thickness. When the slope is very steep the change in feature position with layer thickness change will be small.

To use the performance envelope function, first select the layer for which the performance envelope is to be calculated (select the layer by clicking in the gray box at the left end of the layer). Now select **Performance Envelope** from the **Analysis** sub-menu of the **Tools** menu. A dialog box will appear that allows you to adjust the parameters for the performance envelope calculation. After setting the parameters, click **Plot** to display a graph or click **Table** to show a table of values.

Stress...

Stress is an exceedingly complex phenomenon and we have no models that can attain the same level of success as the model use for the prediction of the optical properties of a coating. This tool makes predictions of stress and strain levels based on a very simple thermal model. Details of different aspects of the model will be found in:

Klockholm, Erik, *Delamination and fracture of thin films.* IBM Journal of Research and Development, 1987. **31**(5): p. 585-591.

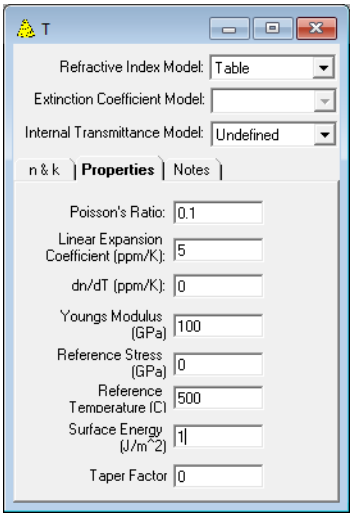
Suhir, E, *Predicted thermally induced stresses in, and the bow of, a circular substrate/thin-film structure.* Journal of Applied Physics, 2000. **88**(5): p. 2363-2370.

Klein, Claude A, *Normal and interfacial stresses in thin-film coated optics: the case of diamond-coated zinc sulfide windows.* Optical Engineering, 2001. **40**(6): p. 1115-1124.

The substrate is assumed to be in the form of a circle of uniform thickness and to be dominant, in much the same way as in the model of optical properties as a function of temperature. A change in temperature causes a change in the dimensions of the substrate according to its coefficient of expansion. The change in the lateral dimensions are impressed on the films, which have themselves changed their dimensions according to their expansion coefficients. Any difference in the coefficients leads to a strain in the films that, by use of Young's Modulus and Poisson's Ratio, can be translated into a biaxial stress. This biaxial stress is added to any intrinsic stress already possessed by the films at the deposition temperature. For this stage of the stress calculation, each film is considered to be independent of any other. The resultant stress, due to all films, acts on the substrate in a way similar to surface tension or compression, forcing it into a spherical shape that depends on the substrate dimensions and material properties. A uniform biaxial compressive or tensile stress in a film will not cause any shear stress at a supporting interface. The shear force is everywhere balanced by an opposite and equal force that distorts the substrate but applies no shear stress. Any variation in the biaxial stress over the surface, however, will immediately translate into a shear stress. Such

variation is a maximum at the edge of the film. Here the shear stress at any interface is at its peak and can be calculated. The films store strain energy. This strain energy can be dissipated as the energy of freshly exposed surfaces in cracking or delamination. The probability of such an effect rises with the strain energy. If there is sufficient strain energy then the cracking or delamination may occur spontaneously. The initiation of such an event usually requires the existence of a sufficiently large defect that can act as a stress concentrator. In practice such defects tend to be found at the periphery of a coating where the delaminating shear stress is already at a maximum. The intrinsic stress in the model is assumed to be a property of the material and the deposition process. We can imagine that the film condenses with zero strain at a particular film temperature that we can think of as its true deposition temperature. Then the film reaches equilibrium with the substrate. In so doing, it acquires the temperature of the substrate but does not change its lateral dimensions. The intrinsic stress originates from the resulting strain. We can consider the true deposition temperature as an unchanging property of the film material (and its deposition technique) but not of its substrate. Knowledge of this property permits the calculation of the effect of any change in deposition temperature. The tool implements this model. The model is purely elastic and reversible. Plastic behavior is excluded.

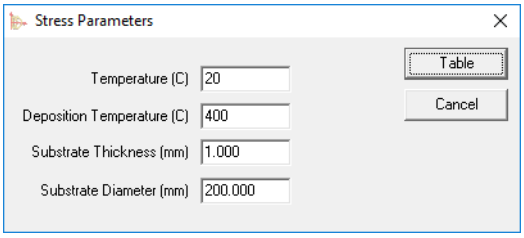
Before the tool can be used, certain data on the thermo-mechanical properties of the layer materials and the substrate must be available. These data are entered in the **Properties** tab of the appropriate material document.



The first two items are shared with the thermo-optical model. The third item is used purely by the thermo-optical models. The lower four items are required for the stress tool. **Young's Modulus** is assumed to be in units of Gigapascals. These units cannot be changed. The **Reference Stress** and **Reference Temperature** are parameters defining the intrinsic stress in the film with sign convention that tensile stress is positive. They are assumed to be measurements of film stress when deposited at the Reference Temperature. Sometimes the stress may have been measured at a measurement temperature different from the deposition temperature. Provided we know the nature of the substrate on which

the measurement was performed, we can derive a corrected Reference Stress by using the tool to model the film on the substrate used for the stress measurement, as though the measurement temperature were the deposition temperature. This procedure will include the necessary correction for the expansion coefficient of the substrate. Note that the temperature is stated as Celsius. The surface energy is used in the calculation of **Cracking Parameter** and **Delamination Factor**. It is rarely known to any great degree of accuracy. Values that can be assumed for glass are around 0.5J/m^2, for metals 1J/m^2 and for high-energy solids like the refractory oxides, perhaps 4 or 5J/m^2. The presence of moisture can actually reduce the high surface energy values by as much as a factor of ten. The increased tendency of coatings to delaminate after humidity testing is well known. Note that surface energies quoted in erg/cm^2 can be converted to J/m^2 using the conversion that 1 J/m^2 = 1000 erg/cm^2.

Once the materials data include the required parameters the tool can be used to examine predicted levels of stress in any design. Selection of **Stress…** in the **Analysis** submenu in **Tools** activates a dialog where some necessary calculation parameters must be entered. The entries in this dialog are stored with the design making it easy to examine the effects of variation of just one of the parameters. The dialog is shown next. The **Temperature** is the temperature at which the stress and the other properties are calculated. **Deposition Temperature** is the temperature at which the films were deposited with their intrinsic stress. **Substrate Thickness** and **Substrate Diameter** are the dimensions of the substrate. The substrate material is that named in the design file.



Stress is calculated by clicking **Table**. The table of results that appears has the following structure.

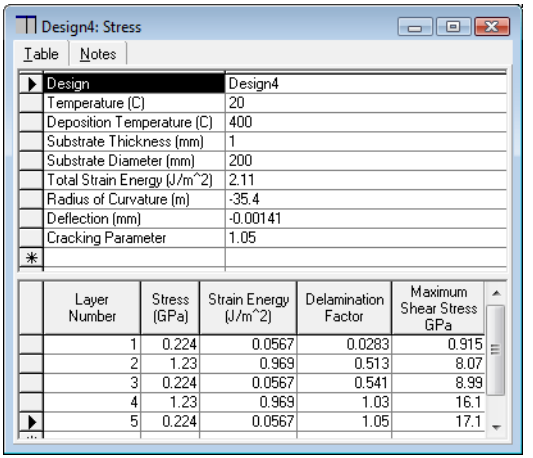

Design4: Stress

Table | Notes

Design	Design4
Temperature (C)	20
Deposition Temperature (C)	400
Substrate Thickness (mm)	1
Substrate Diameter (mm)	200
Total Strain Energy (J/m^2)	2.11
Radius of Curvature (m)	-35.4
Deflection (mm)	-0.00141
Cracking Parameter	1.05

Layer Number	Stress (GPa)	Strain Energy (J/m^2)	Delamination Factor	Maximum Shear Stress GPa
1	0.224	0.0567	0.0283	0.915
2	1.23	0.969	0.513	8.07
3	0.224	0.0567	0.541	8.99
4	1.23	0.969	1.03	16.1
5	0.224	0.0567	1.05	17.1

The upper part of the table exhibits first the input parameters. These are the name of the **Design**, in this case stress test, the **Temperature**, that is the measurement temperature at which the stress is calculated, the **Deposition Temperature** at which the films were deposited and the dimensions of the substrate. Next are four parameters referring to the complete substrate-film combination. The **Total Strain Energy** refers to the total strain energy per unit surface area and includes any intrinsic strain energy. This total energy takes no account of whether or not it is compressive or tensile. In fact there may be a mixture of tensile and compressive strain energy in the layers. This is rather like a spring in compression that maintains a parallel attached spring in tension so that the pair are in equilibrium with no external force. Although the net force is zero the total stored energy is the sum of that in each individual spring. The net stress in the system acts to bend the substrate into a dome. This dome has a **Radius of Curvature** that is positive for a convex coated surface (net stress compressive) or negative for a concave coated surface (net stress tensile). The **Deflection** is the position of the center of the substrate surface with respect to the plane defined by the periphery and indicates the amount by which the substrate departs from its original flatness. The **Cracking Parameter** is an estimate of the ability of the strain energy to supply the required surface energy in a propagating crack that extends through the total thickness of the multilayer. A value of unity means that the two are fairly well balanced. A value of rather less than unity implies a low likelihood of spontaneous cracking while a value elevated above unity suggests that cracking might be a matter for concern. The parameter should be thought of simply as a guide and of course it depends directly on the surface energy figure entered in the film properties.

The lower part of the table applies to the individual films and their interfaces. Each row refers both to the appropriate film and to its inner interface. The interface in the final row, therefore, is the interface with the substrate. **Stress** in Gigapascal is that in the individual film consisting of the intrinsic plus thermal components. The **Strain Energy** is the contribution of the film per unit coated area. The **Delamination Factor** compares the total strain energy per unit area in the outer films with the total surface energy per unit area that is required to generate the two surface produced in a delamination. The interpretation is similar to that for the **Cracking Parameter**. A factor rather less than unity suggests a diminished probability of spontaneous delamination, unless the adhesion

is particularly poor, while a value in excess of unity is a warning sign. The **Maximum Shear Stress** refers to the periphery of the film and applies to its inner interface. The final figure represents the substrate-film interface.

Scattering

This analysis tool predicts the light scattered by a coating. There are two sub-menu options: 2d calculation and 3d calculation. The 2d calculation estimates the scatter as a function of a single variable and the 3d calculation estimates the scatter as a function of two variables. The model used for estimating the scatter is that developed by J. Merle Elson (see, for example, "*Multilayer-coated optics: guided-wave coupling and scattering by means of interface random roughness*" in J. Opt. Soc. Am. A Vol. 12 No. 4, pp729-742, April 1995).

The model assumes that all surfaces have the same roughness. The roughness on each surface may be correlated or uncorrelated. The roughness is described by four parameters: short-range rms roughness, short range correlation length, long-range roughness and long-range correlation length.

The roughness properties of the layer surfaces are represented by a correlation function which is the sum of an exponential function and a Gaussian function:

$$G(\tau) = \delta_L^2 \exp\left(-\frac{|\tau|}{\sigma_l}\right) + \delta_S^2 \exp\left[-\left(\frac{\tau}{\sigma_S}\right)^2\right]$$

where

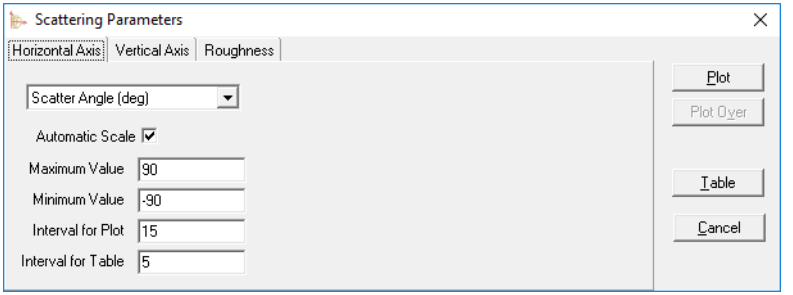
δ_L is the long range rms roughness
σ_L is the long range correlation length
δ_S is the short range rms roughness
σ_S is the short range correlation length

There are two cases for the correlation of roughness between each layer surface: correlated and uncorrelated. Correlated means that the roughness on each surface is identical. Uncorrelated means that the roughness on any layer surface is statistically independent of the roughness on any other layer surface. All layer surfaces use the same statistical parameters defined above for their roughness properties.

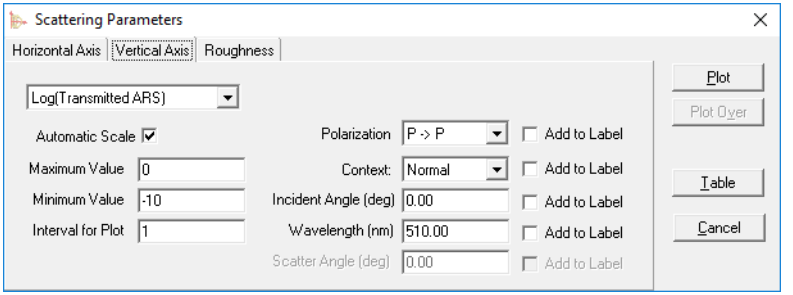
In purely surface scattering into the plane of incidence (the plane containing the incident beam direction and the surface normal), p-polarized incident light induces purely p-polarized scattered light, and, similarly, s-polarized incident light produces purely s-polarized scattered light. Most measurements of the angular distribution of scattered light concentrate on such scattering in the plane of incidence. The tool calculates both polarizations in this plane. For scattering out of the plane of incidence, this rule is no longer true, and there can be mixing of the polarizations. The tool, therefore, also includes two special cases of scattering out of the incident plane into the opposite polarization. This scattering is calculated in a plane normal to the plane of incidence and either from incident p-polarization to scattered s-polarization or incident s-polarization into scattered p-polarization.

For the calculations, the incident angle, scatter angle and wavelength must be specified. For 2d calculations, one of these three parameters will be varied over a defined range and the other two will be held constant. For the 3d calculations, two parameters will be varied over defined ranges and one will be held constant. The calculated result is the Angle Resolved Scatter (ARS). This is given as the ratio of scattered power per unit solid angle to incident power. Either ARS or log(ARS) can be plotted.

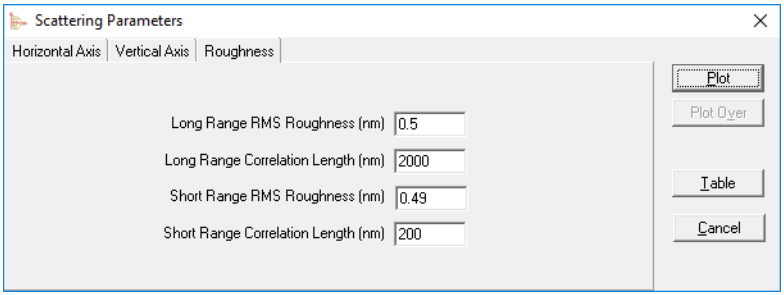
Selecting the 2d calculation option displays the following dialog:



The Horizontal Axis specifies the independent variable for the calculation and the range over which it is to vary.



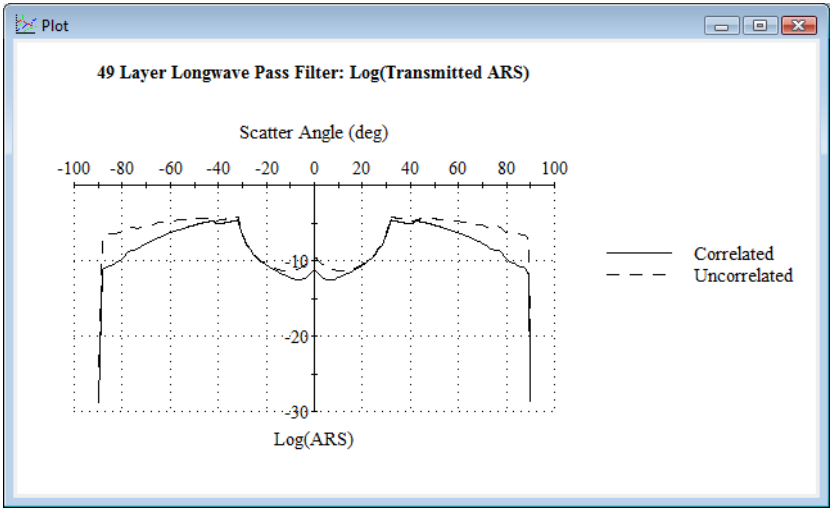
The Vertical Axis tab specifies the scatter output to be plotted. This may be the transmitted scatter or the reflected scatter and whether the ARS or its logarithm is plotted. The polarization parameter controls the polarization state of the incident beam and output scatter beam. There are four possible options: P ->P, P -> S, S -> S, and S -> P. P -> P means that the input beam is p-polarized and the calculations are performed for a p-polarized output beam in the plane of incidence. S -> S is similar except that both beams are s-polarized. P -> S means that the input beam is p-polarized, and the calculations are performed for an s-polarized output beam. The plane of the output beam is 90 degrees to the plane containing the incident beam, the plane of incidence. S -> P is similar except that s-polarization is incident and p-polarized scattered light is calculated in the plane at 90 degrees to the plane of incidence.

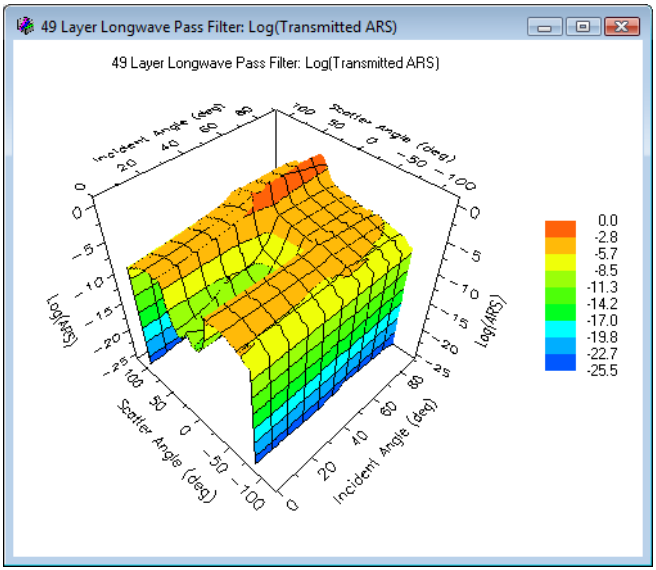


The Roughness tab specifies the statistical properties of the surface roughness. Clicking Plot causes a plot of both the correlated and uncorrelated scattering to be produced for the design.

The first of the following plots shows the calculated scatter for the 49 layer longwave pass filter with a p-polarized 600nm input beam at normal incidence.

Selecting the 3d calculation displays a dialog with similar options except that two independent axes may be specified. The second figure below shows the same calculation but including variation in incident angle.





Design Tools Submenu (Design)

The **Design Tools** submenu has four options. **Edge Filter...**, **Equivalent Layer...**, **Induced Transmission Filter Design...** and **Symmetrical Periods**…. These assist in creating designs for certain specific types of coating.

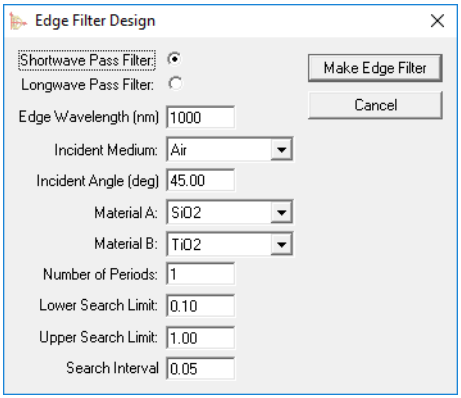
Edge Filter...

Edge filters based on quarterwave stacks show quite large polarization splitting at elevated angles of incidence and, indeed, this behavior is used in the construction of plate polarizers. Conventional edge filters can be considered to be based on a series of symmetrical periods [see **Equivalent Layer...** for more details on symmetrical periods] of form (0.5HL0.5H) or (0.5LH0.5L). No amount of adjustment of relative thicknesses of high and low index materials in such stacks will eliminate the polarization splitting, although it can be slightly varied. The next most complicated symmetrical period based on two materials is of form (aAbBcAbBaA) where A and B indicate high and low index material or vice versa. Such symmetrical periods do include the possibility of elimination of polarization splitting by relative adjustment of the factors a, b and c. Although symmetrical periods with greater numbers of layers are also capable of adjustment, the best performance is usually to be found with the five-layer period. **Edge Filter...** is an option for the automatic design of such symmetrical periods.

Because the edge filter design will be placed in the active design window, overwriting whatever design is already there, the first operation in the design of a completely new filter should always be to activate a new design window by choosing **New...** from the **File** menu. Then select the **Edge Filter...** option. The Edge Filter Design dialog box appears.

Most of the items that are required are obvious. The bottom three require further explanation. There are eight possible configurations [although the solutions may not be distinct] but no analytical expression for the solutions which must be found by an

automatic search of a region. Once a solution is found it can be assessed both in terms of the width of the rejection zone and the width of the pass region. A merit function that is a simple combination of these two attributes allows solutions to be compared and the best selected. No account is taken of the equivalent admittance in the pass region which controls the amplitude of the ripple in the raw design. The three parameters control the width of the search region and the search step. [It is difficult to define exactly the search parameter. It is, in the first instance, the value a of the multiplication parameter for the outermost layers. But then for each value of a, a value of b has to be found that will make the edges for both polarizations coincide. Then all three parameters a, b and c must be scaled to make the edge coincide with the reference wavelength.] The upper limit must be greater than the lower limit but not greater than 2. The lower limit is constrained to be in the range 0 to 1. The search step must be in the range 0.0001 to 1 but the smaller the search step the longer the search takes. A value of 0.05 with a search region of 0.1 to 1 is usually quite adequate. Increasing the range to 0 to 2 is usually ineffective because the solutions that are included in the extra region are normally of the type (.5cAbB2aAbB.5cA).



Once these parameters are entered, the calculation can be launched. A short delay (depending on the range and interval set for the search) follows and then the new design is entered in the design table. Simultaneously, a formula is entered in the formula dialog box so that it can subsequently be used as the core of a more complicated filter.

An example may help. Select a new design and then activate the Edge Filter Design dialog box. Complete the parameters exactly as in the example above. This is an edge filter that is to be matched for 45° in air and is composed of SiO2 and TiO2. It is to be a shortwave pass filter and the edge is at 510nm. The substrate will be glass, although this does not affect the design process and, in fact, the substrate will be whatever is currently listed in the active design window. Next click the **Make Edge Filter** button. After a short pause while the calculations are performed, the design window rapidly fills with the new design.

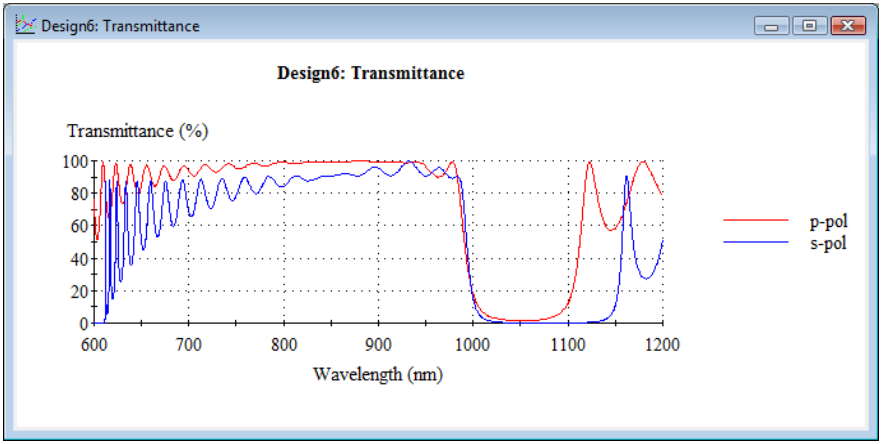
Design6

Design | Context | Notes

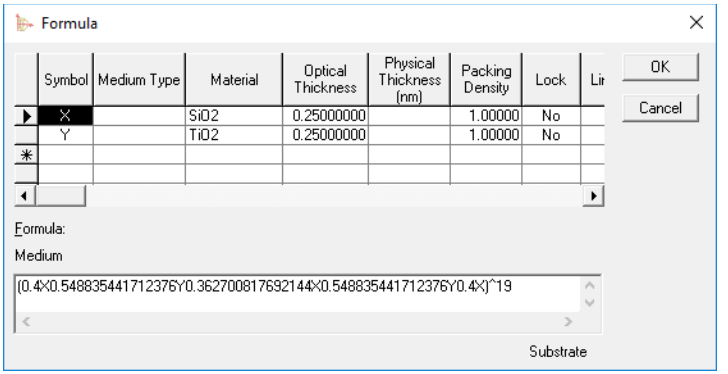
Incident Angle (deg)	45.00
Reference Wavelength (nm)	1000.00

	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
▶	Medium	Air	1.00000	0.00000		
	1	SiO2	1.45044	0.00000	0.10000000	68.94
	2	TiO2	2.25000	0.00000	0.13720886	60.98
	3	SiO2	1.45044	0.00000	0.09067520	62.52
	4	TiO2	2.25000	0.00000	0.13720886	60.98
	5	SiO2	1.45044	0.00000	0.20000000	137.89
	6	TiO2	2.25000	0.00000	0.13720886	60.98
	7	SiO2	1.45044	0.00000	0.09067520	62.52
	8	TiO2	2.25000	0.00000	0.13720886	60.98
	9	SiO2	1.45044	0.00000	0.20000000	137.89
	10	TiO2	2.25000	0.00000	0.13720886	60.98
					10.73676558	6125.01

To calculate the performance of the design, first make sure that both planes of polarization are required at an angle of incidence of 45°. Then select **Plot**. The result is shown below.



With the design window active, select **Formula...** in the **Edit** menu. The Formula dialog box shows the formula.



The option does not consider the ripple performance of the filter at all. Usually, for a shortwave pass filter in the visible and/or near infrared, the outer layer should be of low index. However the resulting design can readily be refined to improve the ripple performance. This is most easily performed with only a few layers unlocked on either side of the multilayer.

Equivalent Layer...

The product matrix of a symmetrical series of layers can be put in the form of the matrix of a single layer. This equivalent single layer possesses the attributes known as the equivalent optical admittance and equivalent phase thickness of the symmetrical system. These attributes may also be known as the Herpin equivalents after the name of an early pioneer. The equivalence is not a physical one but is limited to only those operations that involve multiplication of the characteristic matrices of the layers. In particular it cannot be used to represent the tilted behavior of the coating. The equivalence does, however, extend to absorbing layers but has not been much used for absorbing coatings. Here we are concerned with dielectric layers only. The advantage of this technique is that structures consisting of repeated symmetrical periods of the same kind behave simply as thicker thin films of the same equivalent admittance. Because the symmetrical system is often repeated many times in a single design it is frequently referred to as a symmetrical period, or sometimes a Herpin period.

Equivalent Layer... calculates the equivalent admittance, E, and equivalent phase thickness, γ, of any symmetrical series of dielectric (i.e. transparent) layers. The layers are specified, as normal, by a material and a thickness and the program strips off any extinction coefficient before making the calculations. The module also ignores any angle of incidence that may be entered. Only the normal incidence equivalent parameters are calculated.

The equivalent admittance and phase thickness exhibit regions where they are both real and regions where they are both imaginary, but with dielectric materials there are no regions where one is real and the other imaginary. The real regions correspond to dielectric behavior and it is these regions that are plotted or tabulated. Regions where the equivalent parameters are imaginary are ignored. In these regions of imaginary equivalent

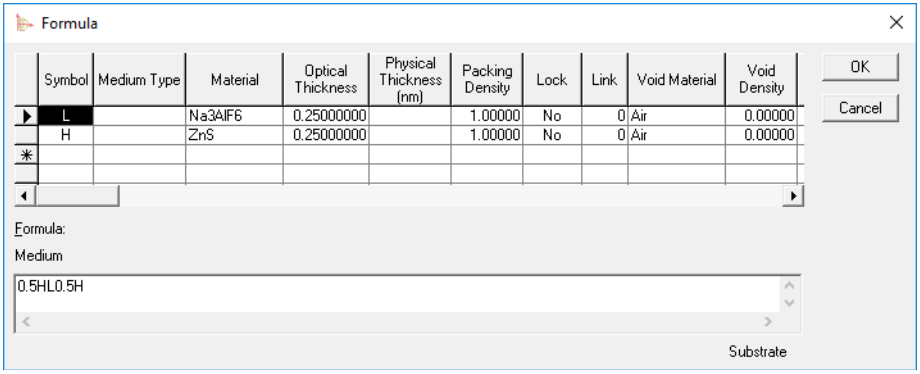
constants the assembly behaves like a metal rather than a dielectric and as the symmetrical period is repeated in the design, the reflectance rises towards 100%.

The equivalent phase thickness, γ, is multi-valued and the value chosen is that closest to the total phase thickness of the original symmetrical period. γ is dimensionless but like normal phase thicknesses it is most readily interpreted if in units of π radians. The units of γ are therefore π. For example when the vertical scale of the plot shows a value of 1.0 for γ then the actual dimensionless value of γ is π.

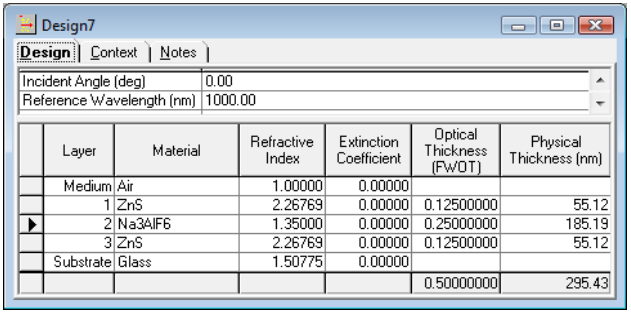
A simple example should help to make the operation clear.

The symmetrical period concerned is specified as a selected series of layers in a design. The design may have additional layers but the calculation will be concerned only with those layers that are selected.

First, with the design window active, select Formula and in the dialog box enter the details shown.

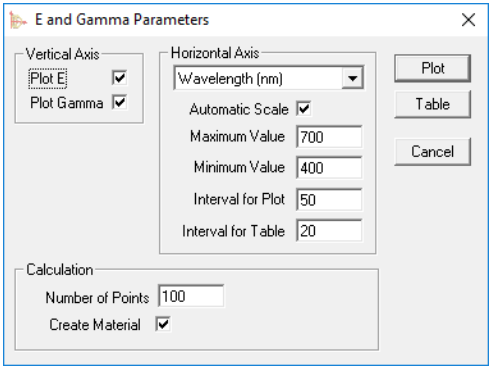


This should give the corresponding design shown below.



Select the three layers by first placing the mouse over the selection box of layer 1. This is the small square cell at the extreme left-hand side. Click once in the box to select the layer. With the shift key depressed, repeat the operation in the selection box of layer 3. This should highlight all three layers. Now, from the **Tools** menu, select **Design Tools**

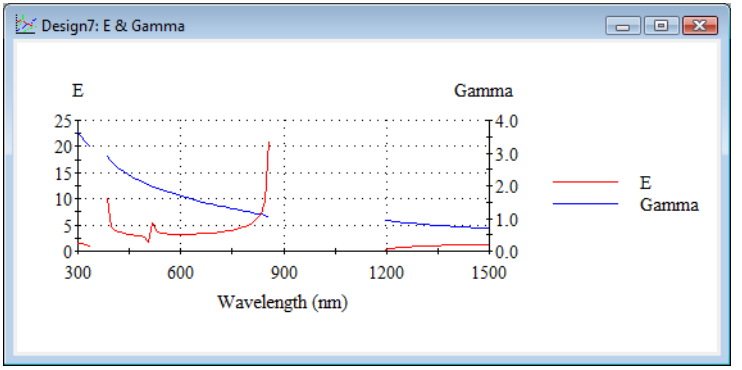
and, finally from the submenu, **Equivalent Layer....** The dialog box that appears is shown next.



This will select either a table or a plot. In either case the imaginary results will not be recorded. Let us choose a plot because that will be easier to interpret.

The number of points is preset at 100 but can be altered as required. The horizontal axis is wavelength and that must be specified. The vertical axis or axes are automatically determined but can be changed later by the Edit commands.

Enter the values shown in the box above and then select Plot. The curves are reproduced below. The gaps in the two curves represent regions where the parameters are imaginary and therefore potential high reflectance zones.

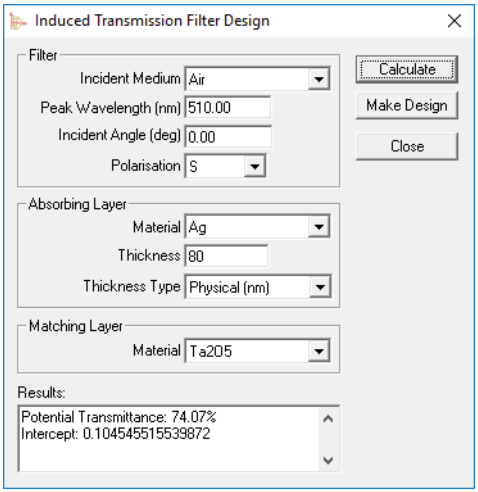


When **Create Material** is checked, a Material window populated with the optical constants of the equivalent material will appear.

Induced Transmission Filter Design...

This option calculates design parameters of induced transmission filters. The user is prompted to enter the details of the absorbing layer followed by the dielectric layers to be used on either side of the absorbing layer. The program then displays the optimum admittance required at the rear (exit) interface, the potential transmittance and the thickness of the matching layer required on either side of the absorbing layer. To complete the matching, the combination of matching layer / absorbing layer / matching layer should be treated as a slab of material of the real admittance given by the entry Intercept (so called because it is given by the intercept of the admittance locus with the real axis). This can readily be achieved by a series of quarterwave layers.

The selection of the menu item activates a dialog box that asks for the input information. The peak wavelength of the filter, the incident medium material, the incident angle and the polarization are asked for first. The polarization may be set either to s or p should the incident angle be non-zero. Note that the incident angle is measured in the incident medium. Even if there is to be a cover cemented over the filter, if the incident angle is ultimately referred to air then that should be entered rather than glass. Next the details of the absorbing layer, that is the material and the thickness are required. This is the layer that is to have maximized transmission. Finally the material for the matching layer must be entered. This material will be assumed perfectly dielectric. Any extinction coefficient will be stripped off before the calculations are performed. Finally, calculations are initiated by pressing the **Calculate** button.

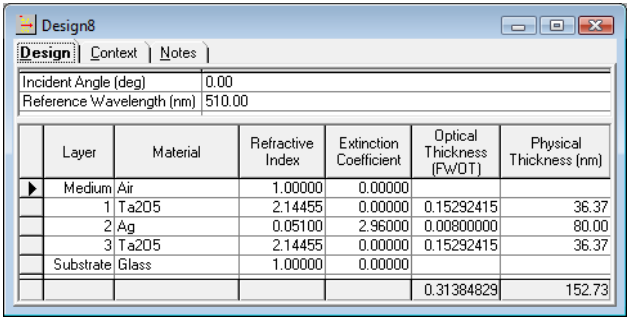


The results are shown in a scrolling text box. The peak wavelength and the reference wavelength are considered to be the same. The optimum exit admittance and the potential transmittance are both listed. Note that the optimum exit admittance will normally be in the first quadrant. Finally the details of the matching layer are displayed, the optical thickness and the intercept. The optical thickness is referred to the peak wavelength as reference. The intercept is the admittance on the real axis, where, either the locus of the matching layer must start, if the optimum exit admittance is to be achieved by the given

phase thickness, or the locus of the matching layer added to the front surface of the absorbing layer must terminate. The results in the text box can be copied to the clipboard by selecting them with the mouse and pressing **<Ctrl>+C**. In this particular case they are:

Potential Transmittance: 74.07%
Intercept: 0.104545
Absorbing Layer n: 0.0510
Absorbing Layer k: 2.9600000
Physical Thickness: 80.000000
Optimum exit admittance: 0.31707 + i3.04661
Matching Layer Refractive Index: 2.1445
Optical Thickness: 0.15292420

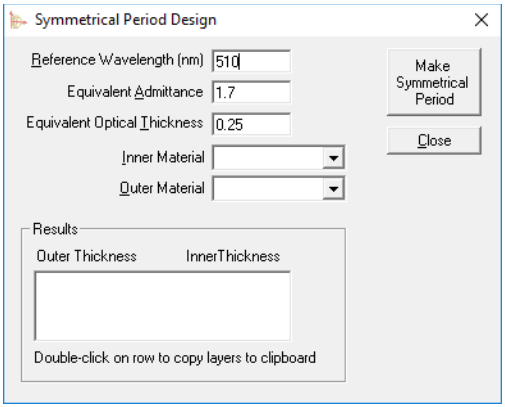
The **Make design** button transfers the results into the active design file but the results do not appear until the **Close** button is clicked (see below). The design will be completed in the usual way by the addition of an appropriate series of quarterwaves between the incident medium and layer 1 and between layer 3 and the substrate.



Symmetrical Periods Design...

It can be readily shown that any combination of thin films which is symmetrical, that is one in which the sequence of layers is unchanged when they are listed in reverse order, can be represented by a single equivalent film having an optical admittance and phase thickness which can be calculated from the parameters of the individual layers. The symmetrical periods design tool will calculate the thicknesses of a 3-layer symmetrical period so that its equivalent film has a desired optical admittance and phase thickness.

The tool is available, when a design window is active, by selecting **Symmetrical Periods** from the **Design Tools** sub-menu of the **Tools** menu. When selected, the following form is displayed.



A symmetrical period is constructed by entering the details of the equivalent layer and then clicking the **Make Symmetrical Period** button. If a symmetrical period can be constructed, then the layers of the symmetrical period will be placed on the clipboard ready for pasting into a design and the window will be closed.

The equivalent layer properties are specified by the **Equivalent Admittance** and **Equivalent Optical Thickness** fields. The **Reference Wavelength** field specifies the wavelength at which the equivalent layer properties are desired. The **Inner Material** specifies the material to be used for the middle layer of the 3-layer structure. The **Outer Material** specifies the material to be used for the first and last layers of the 3-layer structure.

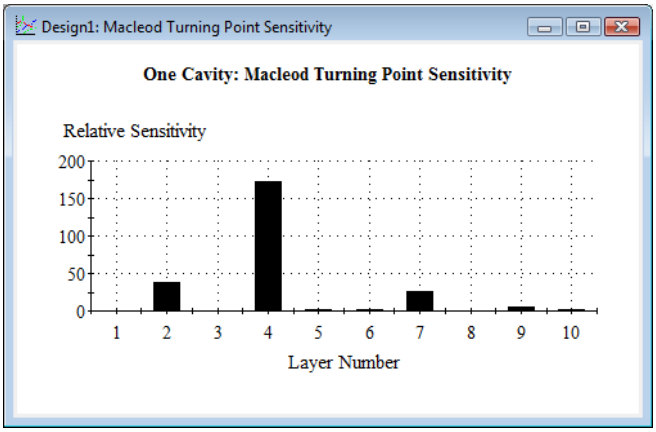
The tool treats all materials as dielectric, that is, any extinction coefficient associated with either of the two materials will be ignored. After clicking **Make Symmetrical Period**, the Results box will be filled with the solutions. Double-clicking on a solution will copy the layers to the clipboard ready for pasting into a design.

Sensitivity Submenu (Design)

The tools in this submenu calculate the sensitivity of a design to various kinds of error. Three types of sensitivity can be calculated: Macleod Turning Point, Independent and Distribution. Note that the Macleod Turning Point sensitivity applies exclusively to a series of quarterwaves or exact multiples of quarterwaves. The results will be meaningless if some layers are of non-integral thickness.

Macleod Turning Point

The Macleod Turning Point sensitivity analysis provides a measure of how difficult each layer in a design is to manufacture. Macleod Turning Point displays a graph showing how critical each layer is in meeting the final transmittance or reflectance magnitude at the reference wavelength. Larger values mean that the production of the layer will be more difficult. For more information on the calculation method see “Turning value monitoring of narrow-band all-dielectric thin-film optical filters” in Optica Acta 1972 Vol. 19 No. 1 pp1-28. The implementation in the Essential Macleod removes the sign and so all values will be positive.



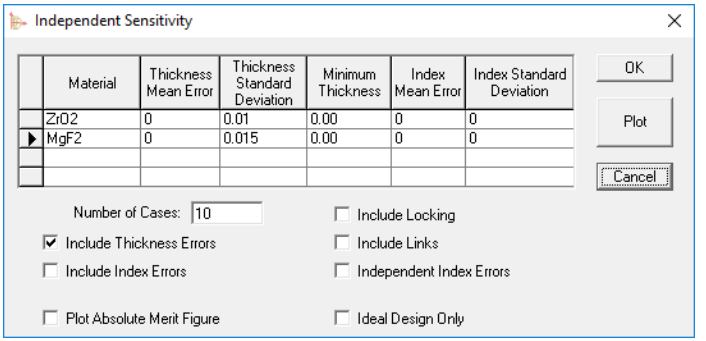
The picture above shows the Macleod Turning Point Sensitivity for a small single cavity filter design for infra-red applications. The chart shows that the most sensitive layer in terms of achieving the desired transmittance at the reference wavelength is the low index layer that is deposited after the cavity. The layer next to the incident medium (layer 1 in the chart above) does not have a sensitivity value because the sensitivity calculation for a layer requires the refractive index of the next layer to be deposited.

The Macleod Turning Point Sensitivity only produces correct results for layers that are an integer multiple of one quarterwave thick. It is acceptable for a design to have, say, an antireflection coating as the first few layers next to the substrate followed by quarterwave layers followed by non-quarterwave layers. The sensitivity results will only be valid for the quarterwave layers.

Independent

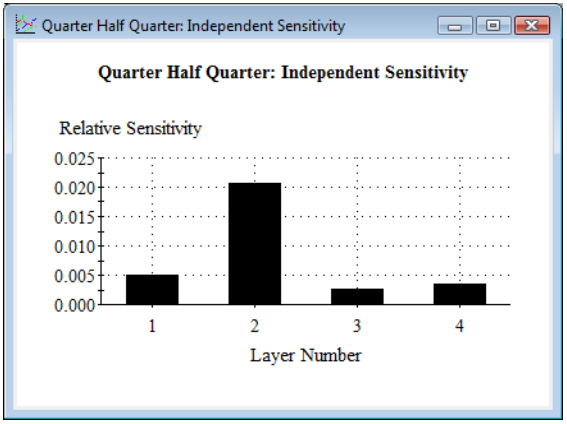
The Independent sensitivity analysis is a Monte Carlo method of assessing the sensitivity of each layer to thickness or refractive index errors. The tool generates a set of designs with errors according to the supplied error parameters. The merit figure of each design is calculated (using the refinement targets) and normalized by taking the Merit Function Power'th root of the merit figure (the Merit Function Power is specified in the refinement parameters). The tool produces one of two kinds of plots. If Plot Absolute Merit Figure is checked then the minimum, lower quartile, upper quartile and maximum merit figures for each layer are plotted. Otherwise it plots, for each layer, the difference between the upper quartile merit figure and the lower quartile merit figure. The larger this number, the more sensitive the layer is to errors.

The Independent sensitivity analysis uses the same error parameters as the Errors tool (see page 92) and has an extra parameter Ideal Design Only. If Ideal Design Only is checked, the sensitivity is calculated by taking the original design and randomly altering each layer Number of Cases times. The plot is then generated from these results.

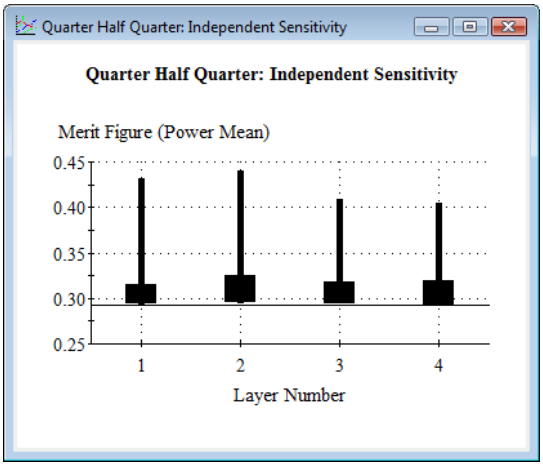


When a coating is manufactured it is very unlikely that all the layers except one will have the correct thickness and refractive index. When Ideal Design Only is not checked, the analysis models this situation by first creating a design where all the layers have been perturbed according to the error parameters. Each layer is then perturbed Number of Cases times. The normalized merit figures are stored for each layer perturbation. This process is repeated so that a total of Number of Cases designs are created and each layer in each of these designs is perturbed Number of Cases times. This process takes more time than the ideal design only case, but gives a more robust indication of the sensitivity of the design.

The figure below shows a sample plot when Plot Absolute Merit Figure is not checked.



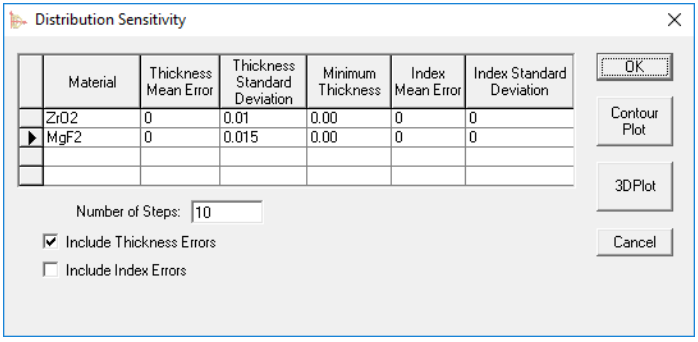
The figure below shows a sample plot when Plot Absolute Merit Figure is checked.



The horizontal line shows the normalized merit figure of the ideal design. For each layer, the top and bottom of the lines show the maximum and minimum merit figures, and the top and bottom of the rectangles show the upper and lower quartile merit figures.

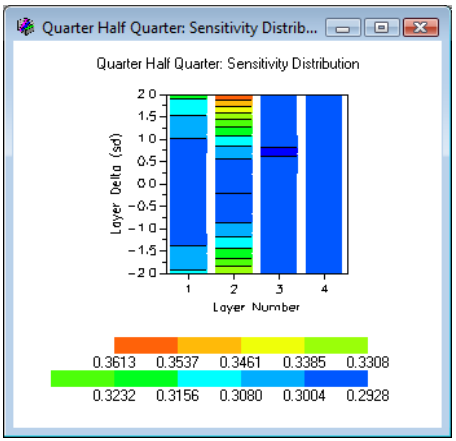
Distribution

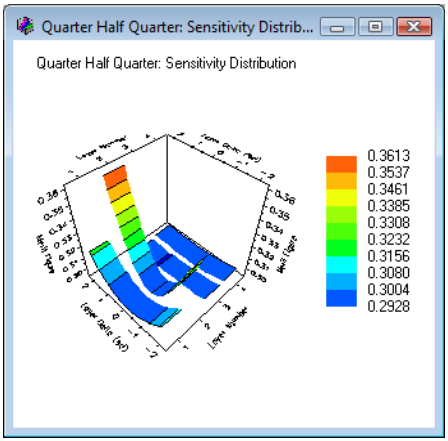
The Distribution sensitivity analysis displays the variation of the merit figure as each layer is varied in thickness or refractive index. The size of the variation is determined by the error parameters. These are the same parameters as used in the Errors command (see page 92). For each layer the error term is varied from –2 standard deviations to +2 standard deviations. This range is divided into Number of Steps intervals. For each point the Merit Figure is calculated (using the current refinement targets) and normalized by taking the Merit Function Power'th root of the merit figure (the Merit Function Power is specified in the refinement parameters).



The results of these calculations can be plotted on either a contour plot or a 3D plot The figure below shows both kinds of plots for the same 4 layer AR used in the Independent sensitivity example above. These plots show that the sensitivity of the

design is greatest for the second layer. They also show that the design is optimal (within the range of layer variations) since the merit figure only gets worse as the layer thicknesses are moved away from the design values.





REVERSE ENGINEER

Reverse Engineer is a tool to help you determine what was actually manufactured and how it compares to your design. To use Reverse Engineer you need the design that you expected to make and at least one spectrophotometer measurement of the manufactured part or one record of the ellipsometric parameters ψ (psi) and Δ (delta) in reflectance.

Introduction

Reverse Engineer operates by successively refining the desired design with varying constraints determined by the user so that the performance of the design better matches the measured performance of the part.

Reverse Engineer keeps a history of each step performed. You can go back to a previous step and continue working from that step, or you can compare the results of one set of steps with another set to decide if one solution is more likely than another.

There are many reasons why a manufactured part does not provide the expected optical performance. Reasons include random errors in the process, incorrect tooling factors, tooling factor changes with deposition, refractive index variation and incorrect thickness termination. The process of reverse engineering attempts to identify the reason(s) why a part does not have the desired performance by analysis of optical measurements made on the part. Although Reverse Engineer can look at variations in absorption through material models, generally, if materials are absorbing more than usual, then this should be fixed (by, for example, adjusting oxygen flow) before using Reverse Engineer.

The analysis is essentially a controlled optimization of the expected design using the measured optical performance as the targets for the optimization. In Reverse Engineer, the optimization is called *Adjustment.* The design is modified during Adjustment so that its performance better matches the measured performance. Generally, there will be different sets of modifications that can be made to the design that will result in the design's performance being equally similar to the measured performance. This multiple solution problem means that steps have to be taken to control the adjustment so that it is directed to the more likely solutions. A solution that has large random changes to several layers is usually less likely than a solution that has consistent change in the layer thicknesses.

Three basic parameter types are controlled by Reverse Engineer: Layer thickness, Packing density and Layer inhomogeneity. To model consistent changes in the manufactured part, such as tooling factor increasing with deposited thickness, a one, two or three parameter model can used. The Constant model uses a fixed offset and represents situations such as the tooling factor being a different value from the one used by the deposition controller. The Linear model provides a linear function relating the change in the parameter as a function of design thickness. This will represent linearly increasing (or decreasing) parameters. The NonLinear model provides a quadratic function to model non-linear relationships between a parameter and deposited thickness.

Reverse Engineer can also adjust Materials that have been specified using a non-tabular model such as Cauchy, Sellmeier, Drude, Lorentz and Drude-Lorentz. With the Function enhancement, other user-defined material models can be used to specify the

index dispersion properties of a material used in the design. When a material model is used, it calculates the refractive index and extinction coefficient values used by Reverse Engineer. The optical constant data specified by the material in the design is not used. For more information on user-defined material models, see the Material Model section in the Scripting Language Help.

The parameter models can be selectively applied to the different materials used in the design. For example, in a design using SiO2 and TiO2, a Linear model could be applied to SiO2 Layer thicknesses only and the TiO2 may not have any models applied to it. During adjustment, the optimization would attempt to find a solution using only a linear change in SiO2 tooling factor.

For modeling random changes in layer parameters, each parameter type can be allowed to independently vary for each layer. Since the layer parameters vary independently, there is no corresponding model to be applied. The choice is simply to allow a layer parameter to vary or not.

In addition to the adjustment of layer properties, Reverse Engineer also permits the adjustment of the measured data, that is, the wavelength, transmittance and/or reflectance information. This data may only be varied using a one, two, or three-parameter model. For best results, measurements must always be made as accurately as possible on a calibrated and maintained spectrometer. Any errors in measurement will, in general, increase the uncertainty in any results obtained. The adjustment of measured data should only be used as a last resort in attempting to determine the source of the manufacturing errors.

Another source of control over the optimization process is provided by the sequence of adjustments made to the design. In a manufactured part where the errors consist of a tooling factor variation and some small random errors due to noise in the system, the best results are likely to be obtained by first looking for a tooling factor variation that best fits the data, followed by determining how much random variation will complete the fit. The *Action* for each material/layer controls the use of the parameters during adjustment. There are four types of Action available: Not Used, Adjust, Reset & Adjust and Lock. Not Used, means that the parameter does not take part in adjustment and is value is such that the design is not modified by it. Adjust means that the parameter does take part in adjustment and if the parameter has been adjusted in a previous adjustment, the starting point for the next adjustment will be the ending point of the previous adjustment. Reset & Adjust performs the same function as Adjust except that the parameter is reset to its initial value where it did not modify the design. Lock means that the parameter does not take part in the next adjustment, but the parameter retains the value it had at the end of the last adjustment.

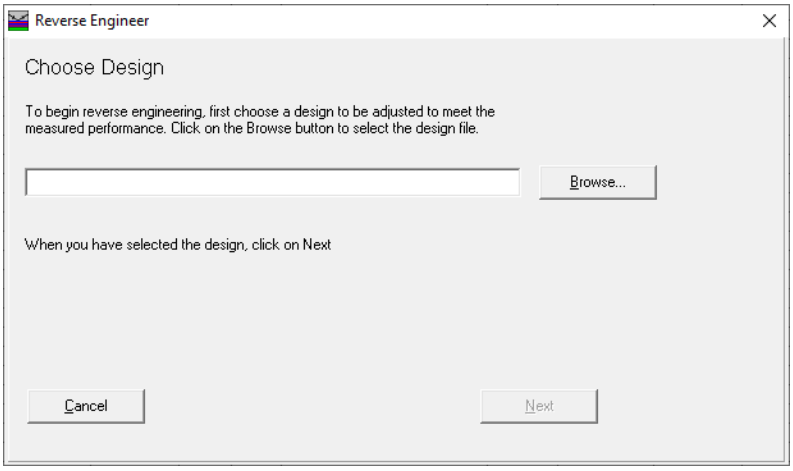
The sequence of adjustments to make the design match the measurements would be: set each material's model order to Linear (to look for a linear tooling factor variation), set each material's action to Adjust, and then adjust the design. At the end of this adjustment, set each material's Action to Lock (to retain the adjusted tooling factor values), set each layer's thickness action to Adjust and then adjust the design. This prevents the tooling factor from changing and provides an estimate of the amount of random variation needed to make the design match the measured data. This can be compared with the expected random variation to see if it is plausible.

If the sequential adjustment and use of Locks were not used, then the adjustment would be free to vary the random thickness parameters by larger values and use less variation in the material's tooling factor. The design could still match the measured data, but the results would be less plausible because of the increased random variation.

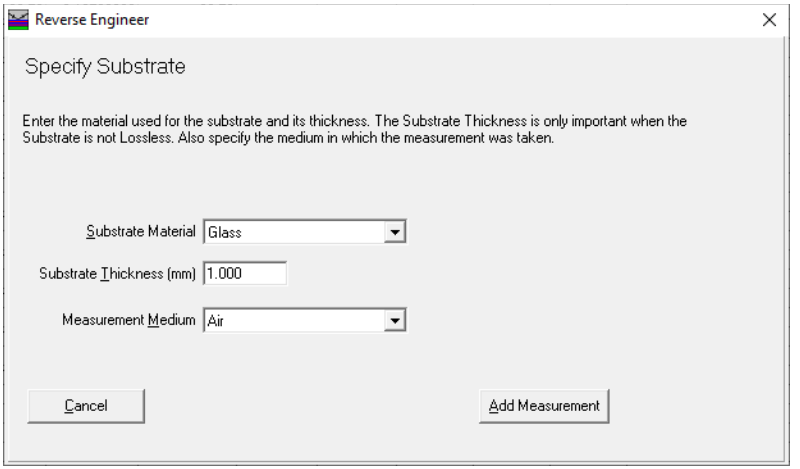
The results of adjustment can be seen in both tabular and graphical form. The design display shows the changes made to each layer by the adjustment process for both the systematic material changes and the random per layer changes. Graphically, the systematic changes can be plotted as a function of deposited thickness. The random changes can also be plotted on bar charts together with the systematic changes.

Operation

To start Reverse Engineer, from the File menu, select New and then Reverse Engineer. A blank Reverse Engineer window will appear together with an initial data window where you can enter information needed to start reverse engineering.

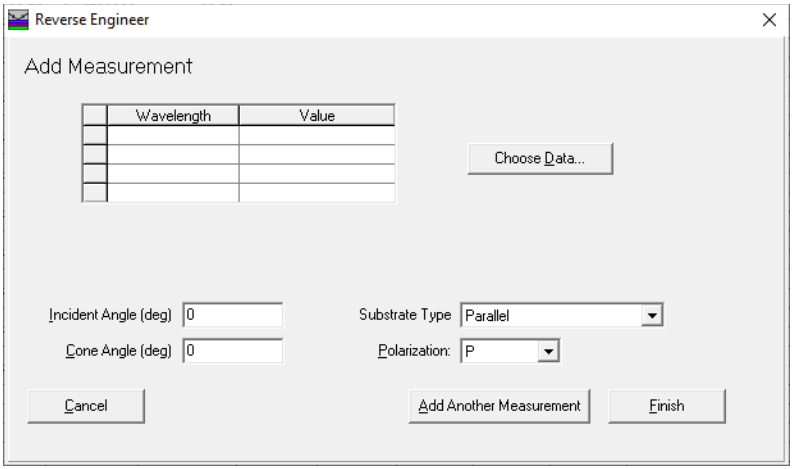


A file chooser will appear so you can select the design file containing the design that was made. If, after having chosen a design, you want to change the design file, click Browse to open the file chooser again. Click Next to continue.



The substrate on which the design was deposited must now be defined. This information will be used instead of the corresponding data in the design file for performance calculations in Reverse Engineer. The Substrate Material is the material file containing the refractive index information and internal transmittance data for the substrate. If the internal transmittance data is undefined in the Material file, Substrate Bulk will be visible and specifies the substrate file containing the internal transmittance data for the substrate. The Measurement Medium is the material file containing the data corresponding to the medium in which the measurements took place. This will usually be Air. The Substrate Type refers to the treatment of multiple beams in the substrate. If all light reflected in the substrate and coating finally impinge on the measuring device's detector, then the Substrate Type should be set to Parallel. If the reflected light does not reach the detector (for example, it leaves the aperture of the system on reflection from the rear surface of the substrate), then the Substrate Type should be set to Wedged. Where reflectance has been measured and the substrate has a ground rear surface or the reflection from the rear surface has been removed by other means, Wedged should also be used to indicate that only the reflectance of the coating has been measured.

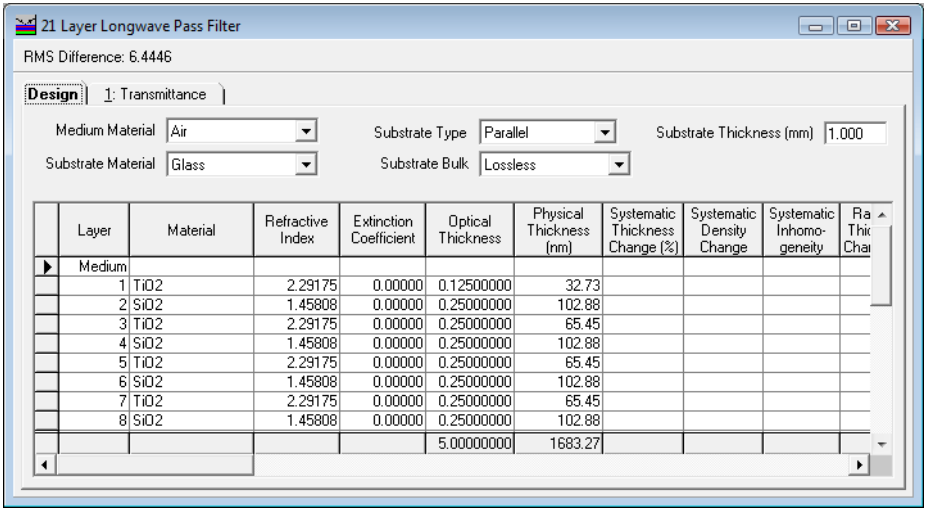
Once this information has been completed, click Add Measurement to add the measurement data.



To add a spectrum, click Choose Data to select the file and specify the wavelength and measurement data to be used. This data will appear in the table to the left of the Choose Data button (the data cannot be edited). The remainder of the form is used to specify the measurement parameters. Incident Angle and Polarization define the angle of the beam with respect to the normal to the coating and the polarization state of the beam. For coatings where the cone angle of the measuring beam has a significant impact on the measurement, enter the cone semi angle of the beam. Substrate Type can be either Parallel or Wedged. These have the same meanings as for Thick Layers in the Design editor. Typically Parallel will be used when second surface effects are included in the measurement and Wedged will be used when the second surface effects have been eliminated by, for example, grinding the rear surface. For normal incidence measurements, the Polarization does not affect the calculations and can be ignored. For oblique incidence magnitude measurements, it is recommended that a p or s-polarized beam is used. The light beam in most spectrometers has more energy in one polarization direction than the other. Using Mean polarization when the beam's polarization is not controlled could lead to additional errors in the results.

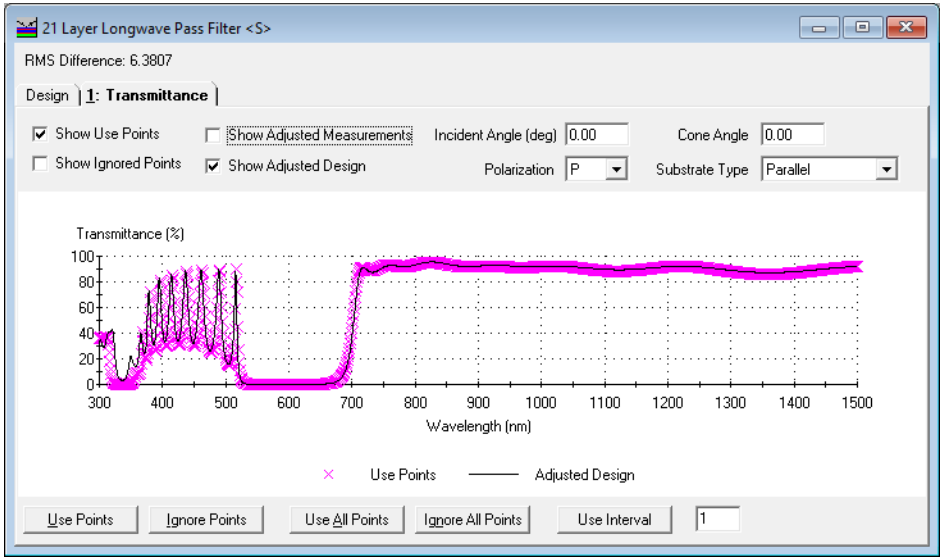
If you have taken more than one measurement, the additional measurements can be added, one at a time, by clicking the Add Another Measurement button.

When the last measurement has been specified, click Finish to exit the data entry stage. The figure below shows the Reverse Engineer window with a design and transmittance measurement loaded.

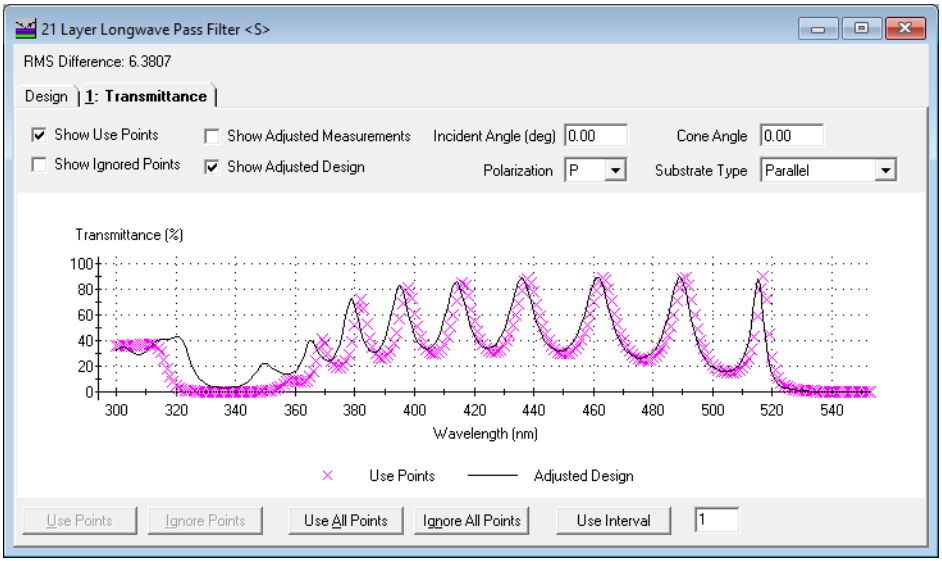


	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness	Physical Thickness (nm)	Systematic Thickness Change (%)	Systematic Density Change	Systematic Inhomo-geneity	Ra Thic Cha
▶	Medium									
	1	TiO2	2.29175	0.00000	0.12500000	32.73				
	2	SiO2	1.45808	0.00000	0.25000000	102.88				
	3	TiO2	2.29175	0.00000	0.25000000	65.45				
	4	SiO2	1.45808	0.00000	0.25000000	102.88				
	5	TiO2	2.29175	0.00000	0.25000000	65.45				
	6	SiO2	1.45808	0.00000	0.25000000	102.88				
	7	TiO2	2.29175	0.00000	0.25000000	65.45				
	8	SiO2	1.45808	0.00000	0.25000000	102.88				
					5.00000000	1683.27				

In the Design section, the details of the design and substrate can be seen. The substrate details can be edited if necessary. The Transmittance section shows the measured performance and that predicted from the design.

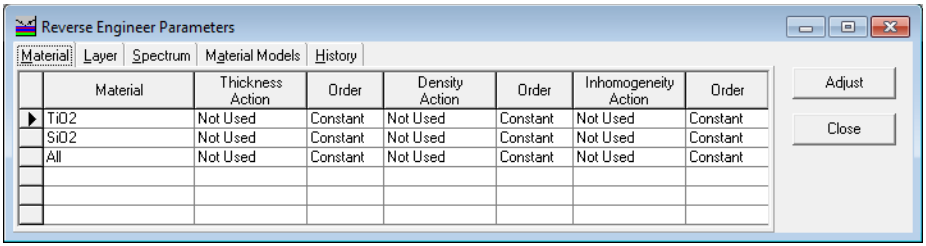


In the figure below, the plot is zoomed to show the differences between the measured data and the predicted performance at the short wavelength end of the plot.



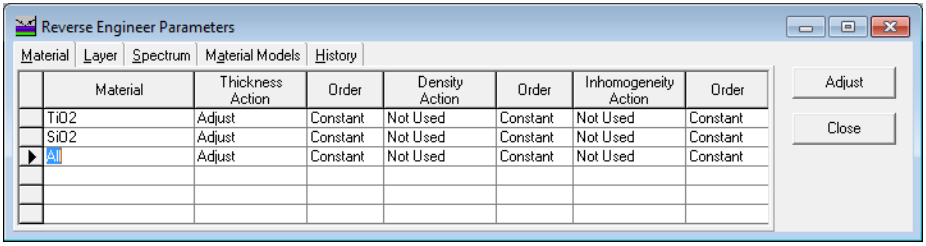
The black line shows the predicted performance and the purple crosses show the measured performance. From the measured data you can select a subset of the data to be used during adjustment. Using a smaller number of data points increases the speed of adjustment, but sufficient data points need to be used to ensure that the shape of the predicted curve cannot be substantially different to the measured curve and still match all the selected data points. The check boxes Show Use Points and Show Ignored Points show you points which will be used in adjustment and which points will not. The purple colored points are used in adjustment and the blue colored points will be ignored during adjustment. To select a range of points, drag a box around the points. Click Use Points to mark the selected points as used during adjustment. Click Ignore Points to mark the select points as ignored during adjustment. You can also select Use All Points to put all the measured data points into the set to be used for adjustment or Ignore All Points to remove all the points from the set used for adjustment. After using Ignore All Points, you will need to add some points before adjusting the design. Finally, Use Interval is used in conjunction with the box to the right of the button. Enter a whole number into the box and click Use Interval. If you entered 10, every tenth point will be added to the set used for adjustment and all other points will be removed from the set.

The top of the window shows the RMS difference between the measured data points and the predicted data points. If the data points match perfectly, this value will be zero. From the Adjust menu, click Parameters. The adjustment parameters window will appear in the bottom right corner of the Essential Macleod window. You can move the window to a different location if you wish. This window is used to select the kinds of changes that will be permitted during adjustment.

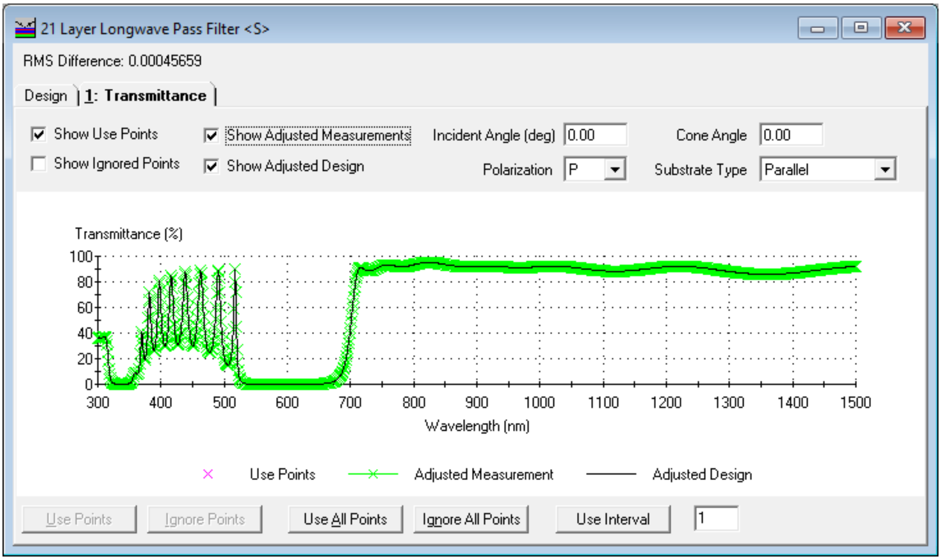


The parameters window has five sections: Material, Layer, Spectrum, Material Models and History are available. The Material section is used to specify the systematic changes that can be made to the design. The changes are specified per material used in the design. For convenience, the last row labeled All can be to set the same parameter for all materials. The Layer section is used to control the adjustment of each layer independently of the other layers. The Spectrum section is used to control the adjustment of the spectra. The Material Models section is used to define which materials will use a model rather than the material data specified in the Design. This section is also used to create material data from the adjusted model that can be stored in the materials database. The final section, History, provides a record of the adjustments made to the design.

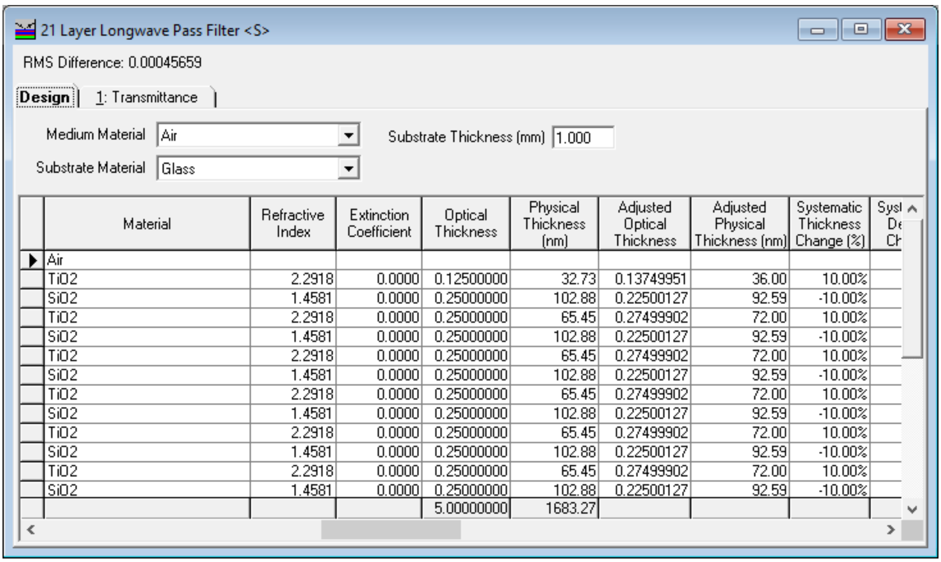
One reason for production errors is incorrect tooling factor. The Thickness Action and Order in the Material section can be used to search for incorrect tooling factor. To search for a constant offset in tooling factor, change the thickness action in the All row to Adjust. The Order should be left at Constant.



Click Adjust to begin the adjustment. The RMS difference value will be updated as the adjustment progresses. To show that the adjustment is running a bar to the right of the RMS value will appear and change in size. At the end of adjustment, the bar will disappear. The plot is only updated at the end of adjustment as shown in the figure below.

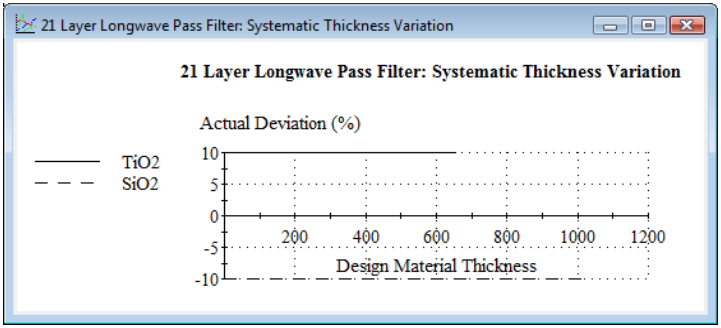


The match between the measured data and the modified prediction is now so good that there is no value in attempting to improve the match. We can now look at the results of the adjustment. We can see the results in terms of changes to the layers by selecting the Design section of the window as shown below. The Systematic Thickness Change column shows that the TiO2 layer thicknesses have been increased by 10%, and that the SiO2 layer thicknesses have been decreased by 10%.

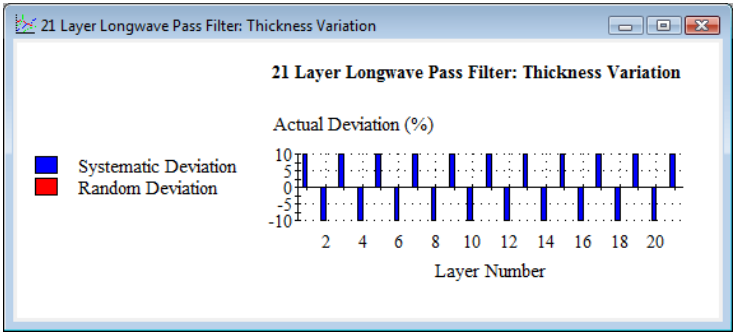


Material	Refractive Index	Extinction Coefficient	Optical Thickness	Physical Thickness (nm)	Adjusted Optical Thickness	Adjusted Physical Thickness (nm)	Systematic Thickness Change (%)	Syst De Ch
Air								
TiO2	2.2918	0.0000	0.12500000	32.73	0.13749951	36.00	10.00%	
SiO2	1.4581	0.0000	0.25000000	102.88	0.22500127	92.59	-10.00%	
TiO2	2.2918	0.0000	0.25000000	65.45	0.27499902	72.00	10.00%	
SiO2	1.4581	0.0000	0.25000000	102.88	0.22500127	92.59	-10.00%	
TiO2	2.2918	0.0000	0.25000000	65.45	0.27499902	72.00	10.00%	
SiO2	1.4581	0.0000	0.25000000	102.88	0.22500127	92.59	-10.00%	
TiO2	2.2918	0.0000	0.25000000	65.45	0.27499902	72.00	10.00%	
SiO2	1.4581	0.0000	0.25000000	102.88	0.22500127	92.59	-10.00%	
TiO2	2.2918	0.0000	0.25000000	65.45	0.27499902	72.00	10.00%	
SiO2	1.4581	0.0000	0.25000000	102.88	0.22500127	92.59	-10.00%	
TiO2	2.2918	0.0000	0.25000000	65.45	0.27499902	72.00	10.00%	
SiO2	1.4581	0.0000	0.25000000	102.88	0.22500127	92.59	-10.00%	
			5.00000000	1683.27				

Alternatively, the tooling factor as a function of design thickness can be plotted. With the Reverse Engineer window selected, select Systematic Thickness from the Results menu. The scaling factor will be plotted.



Another output format, which has more value when there are random variations, is a bar chart of the changes. From the Results menu, select Random Thickness.



In this case, the bars are all constant length. If there were some random variation as well, red bars to the side of the blue bars would indicate the amount of random variation in comparison to the systematic variation.

Menu Commands

This section describes the menu commands specific to Reverse Engineer.

File Menu

Import

When the Design section is displayed, this command allows you to load a design into Reverse Engineer for adjustment. Generally, this command will not be used, because the design will already have been imported during initial data entry.

Measurements Menu

Add Transmittance

The Add Transmittance command will add a transmittance measurement to the set measurements loaded into Reverse Engineer. When you click this command, you be asked to select the file containing the measurement data. After this, you will be asked to define the wavelength and transmittance column. Finally you have to select the scale range of the transmittance measurement, either 0-1 or 0-100%. The transmittance measurement will appear in a new section of the Reverse Engineer window. In that window you can set the Incident Angle and polarization used for the measurement.

Add Reflectance

Add Reflectance performs the same function as Add Transmittance except that it loads reflectance curves.

Add Reflectance Psi

Add Reflectance Psi performs the same function as Add Transmittance except that it loads reflectance psi curves.

Add Reflectance Delta

Add Reflectance Delta performs the same function as Add Transmittance except that it loads reflectance delta curves.

Delete Measurement

This command removes the measurement in the displayed section from the loaded measurement set.

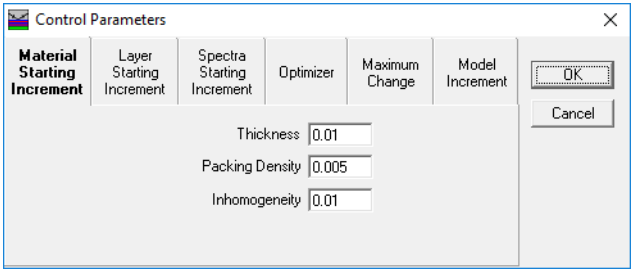
Adjust Menu

Parameters

This command displays the adjustment parameters in a window at the bottom right of the Essential Macleod window. From this window, you control the parameters that are to be used during the adjustment of the design. This window also keeps a history of the adjustments previously made and the RMS difference that was achieved.

Control Parameters

This command provides control over the parameters that limit the adjustment process. These parameters are not normally changed, but occasionally, modifying these parameters will improve the performance of Reverse Engineer.



The following control parameters are available:

Material Starting Increment Section

Thickness: The adjustment process starts by creating a set of designs clustered around the starting point. This value specifies the proportional amount of thickness that is added to the starting point to generate the cluster for thickness values.

Density: This parameter performs the same function as Starting Material Thickness Increment, for the Material Density parameters, except that the value is an absolute amount added to the starting value of packing density..

Inhomogeneity: This parameter performs the same function as Starting Material Thickness Increment, for the Material Inhomogeneity parameters except that the value is an absolute amount added to the starting value of inhomogeneity factor.

Layer Starting Increment Section

Thickness: This parameter specifies the amount of thickness added to the design when creating the initial cluster for random thickness changes.

Density: This parameter specifies the amount of packing density added to the design when creating the initial cluster for random density changes.

Inhomogeneity: This parameter specifies the amount of inhomogeneity factor added to the design when creating the initial cluster for random inhomogeneity changes.

Spectra Starting Increment Section

Wavelength: This parameter specifies the proportional amount of wavelength change made when creating the initial cluster.

Transmittance: This parameter specifies the proportional amount of transmittance change made when creating the initial cluster

Reflectance: This parameter specifies the proportional amount of reflectance change made when creating the initial cluster

Optimizer: General Section

Simplex: When selected, simplex optimization will be used.

Differential Evolution: When selected, differential evolution optimization will be used.

<S> will appear in the title bar when Simplex is chosen and **<DE>** will appear when Differential Evolution is chosen

Optimizer: Simplex Section

Number of Iterations: The maximum number of cycles of simplex optimization before adjustment will halt. If this value is reached, a message will be displayed.

Limiting Range for Merit Function: When the difference between the best and worst performances generated during adjustment is less than this value, the adjustment will stop.

Optimizer: Differential Evolution Section

Number of Iterations: The maximum number of cycles of differential evolution optimization before adjustment will halt. If this value is reached, a message will be displayed.

Merit Function Limit: When the best performance generated during adjustment is less than this value, the adjustment will stop.

Population Scale Factor: This determines the size of the population of candidate designs for the Differential Evolution optimization. The larger this number, the bigger the population size. An increased population size has a better chance of finding a good solution, but at the expense of increased adjustment time.

Maximum Change Section

Thickness: This parameter specifies the maximum change in thickness allowed for the design. This value applies to the combined thickness change from systematic effects and random effects.

Density: This parameter specifies the maximum change in density allowed for the design. This value applies to the combined density change from systematic effects and random effects

Inhomogeneity: This parameter specifies the maximum change in inhomogeneity allowed for the design. This value applies to the combined inhomogeneity change from systematic effects and random effects

Wavelength: This parameter specifies the maximum change in wavelength allowed for the measurements.

Transmittance: This parameter specifies the maximum change in transmittance allowed for the measurements.

Reflectance: This parameter specifies the maximum change in reflectance allowed for the measurements.

Model Increment: Cauchy Section

A: This parameter specifies the default starting increment for the A parameter.

Model Increment: Sellmeier Section

A: This parameter specifies the default starting increment for the A parameter.

B: This parameter specifies the default starting increment for the B parameter.

Model Increment: Drude Section

A: This parameter specifies the default starting increment for the A parameter.

B: This parameter specifies the default starting increment for the B parameter.

C: This parameter specifies the default starting increment for the C parameter.

These defaults apply to both the Drude and Drude-Lorentz material models.

Model Increment: Lorentz Section

A: This parameter specifies the default starting increment for the A parameter.

B: This parameter specifies the default starting increment for the B parameter.

C: This parameter specifies the default starting increment for the C parameter.

D: This parameter specifies the default starting increment for the D parameter.

These defaults apply to both the Lorentz and Drude-Lorentz material models.

Model Increment: k Cauchy Section

A: This parameter specifies the default starting increment for the A parameter of the extinction coefficient Cauchy model.

Model Increment: k Exp Section

A: This parameter specifies the default starting increment for the A parameter of the extinction coefficient exponential model.

B: This parameter specifies the default starting increment for the B parameter of the extinction coefficient exponential model.

Results Menu

This menu provides graphical output of the adjustment results.

Systematic Thickness
Systematic Density
Systematic Inhomogeneity

These three commands display the systematic variations of Thickness, Packing Density and Inhomogeneity for each material on separate plots.

Random Thickness
Random Density
Random Inhomogeneity

These three commands display the random variation and systematic change to each layer in Thickness, Packing Density and Inhomogeneity on separate bar chart plots. The systematic and random changes are shown in separate bars so that their relative sizes may be easily compared.

Spectra

This command plots the variation in the measurement parameters that have been used in the adjustment.

Adjustment Parameters Window

The adjustment parameters window provides the control over the adjustment process.

For each parameter, there are four kinds of action that can be specified: Not Used, Adjust, Reset & Adjust and Lock. Not Used means that the parameter does not modify the design. Adjust means that the parameter is modified by the adjustment process and that the starting point for the parameter is the value it had at the end of the previous adjustment. For the first adjustment, the value of the parameter is such that it does not modify the design. Reset & Adjust is the same as Adjust except that the parameter is reset to its initial value before the first adjustment each time an adjustment is made. Lock means that parameter keeps the value it had at the end of the previous adjustment and is not modified during adjustment.

In the Material and Spectrum sections, an order is also specified for each parameter. The possible orders are Constant, Linear, and NonLinear. A Constant order means that a constant offset that is independent of thickness or wavelength is applied to the parameter. A Linear order means that an offset that varies linearly with thickness or wavelength is applied to the parameter. A NonLinear order means that an offset that varies quadratically with thickness or wavelength is applied to the parameter.

To change the values of the Action or Order, click in the cell until the desired value appears. Once the values have been set, click the Adjust button to begin adjustment of the design. Clicking the Close button will close the Adjustment Parameters window.

Material Section

This section controls the systematic variations applied to the design. For each material used in the design, the thickness, density and inhomogeneity variations are controlled by the order of the model.

At the bottom of the list of materials is the special name All. Changing the parameters of All changes all the material parameters of the same kind to the same value.

Layer Section

This section controls the random variations applied to each in the design. Only the Action can be set since there is no relationship between the changes in layers. At the

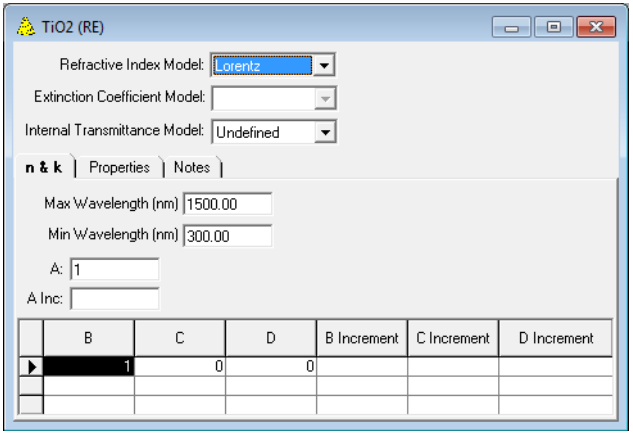
bottom of the layer column is the special name All. Changing the Action in this row makes all the layers have the same action.

Spectrum Section

This section controls the variations applied to the magnitude measurements. The ellipsometric parameters psi and delta cannot be adjusted. Only systematic variations may be applied to the measurements, and the variations are assumed to be consistent across all measurements of the same type. The wavelength can also be modified and the modifications are applied to the wavelengths of all measurements.

Material Models Section

This section controls the variations applied to the materials. Clicking in the Action cell will change how the material is used in adjustment in the same way as for the other parameters. If Function is not present, the then Script Name will show <Internal>. If Function is present, it will be possible to select a script that will provide a material model, otherwise one of the internal material models must be used. If the material already uses a non-tabular model, then this model will used during adjustment. If the material is only defined by a tabular model, then one of the other models must be selected before adjustment. Reverse Engineer does not modify the existing material, but makes a copy of the material and makes changes to the copy. This copy can be edited by clicking the Show button in the Parameters column. This will display a Material window. The name of the Material will be the same as in the Material column with "(RE)" appended. In this window, you can change the material model used and the parameters. In addition to the parameters for the particular material model, there are also the increment parameters. For example, in the Lorentz model, the Material parameters include A Inc, B Increment, C Increment and D Increment:



When these increment parameters are left blank, the default parameters specified in the Control Parameters will be used, otherwise the increments in the material will be used. When the selected optimizer is Simplex, the increments are used in the usual way to add offsets to each parameter to form the initial simplex. When the selected optimizer is

Differential Evolution, the increments are used together with the parameters to create the initial range for each of the parameters: (parameter – increment) to (parameter + increment).

After each adjustment has completed, the Material window can be used to see the current state of the Material definition, by making the Material window active and using the plot commands to view the refractive index dispersion. Between adjustments, the material data can be edited. The new edited data will be used in the next adjustment.

History Section

This section records all the adjustments made to the design. The RMS difference and the parameters used are stored for each adjustment. Double-clicking on an entry in the history will restore the state of Reverse Engineer to that entry. This means that you can easily backtrack to earlier point if you need to try an alternative set of adjustments, but do not need to go back to the beginning.

REPORT GENERATOR

Introduction

The Report Generator is used to make customized printouts of data contained in Essential Macleod files. Data can be printed from associated files as well as the data contained in the file to be printed. For example, the report for a Stack can include listings of the designs used in the Stack. Additionally, the report can include plots and tables, such as the reflectance spectrum of a Design.

A Report is created by applying a Report Template to an Essential Macleod file. To apply a report template to an open Essential Macleod file such as a Design, select either Preview Report or Print Report from the File menu. Selecting Preview Report will cause the report to be displayed in a print preview window. Selecting Print Report will cause the report to be printed on the currently selected printer.

The Report Template describes the format of the printed output and the information to be extracted or calculated by the Essential Macleod. Report template files are text files and can be edited with any text editor as well as being edited by the Essential Macleod. Report template files have the extension .rpx.

The text in a report template is either text that is to be printed directly without interpretation, or it is an instruction that is replaced by data from the Essential Macleod. Instructions begin with the character sequence "%<" and end with the character sequence "%>" For example, a report template file that contains the line

```
%<Design Layers%>
```

when applied to a Design will print out the layers used in the design as they appear on the screen.

Instructions

An instruction consists of a list if items separated by space characters. Where an item contains spaces (such as a font name), it must be enclosed in double-quotes ("), for example, "Times New Roman".

Page Layout Instructions

Page layout instructions control the general features of the page. This includes the orientation of the page and the font used.

%<Portrait%>: Forces portrait orientation of the paper. If a page has been started, this will take effect at the next page

%<Landscape%>: Forces landscape orientation of the paper. If a page has been started, this will take effect at the next page

%<Header *HeaderText*%>: The header is set to be *HeaderText*. This has the same formatting rules as the standard header specified in the options. If this header is not present, then the standard header is used.

%<Footer *FooterText*%>: The footer is set to be *FooterText*

%<NewPage%>: Starts a new page.

%<Font *Parameters*%>: Modifies the font. The parameters are:

Bold

NoBold

Italic

NoItalic

Underline

NoUnderline

StrikeThru

NoStrikeThru

Size: Followed by the size in points

Name: Followed by the font name in quotes

For example

%<Font Arial Size 15%>

sets the font to be Arial at a size of 15 points

%<HeaderFont *Parameters*%>: As for Font but controls the font used for the header and footer.

%<Graphic <Filename> *Parameters*%>: prints the graphic is the specified file on the page. The following file formats are supported: bmp, gif, jpg, wmf (Windows Metafile) and emf (Enhanced Metafile). The following parameters are available:

Width: Specifies the width in inches

Height: Specifies the height in inches

Center: Horizontally centers the graphic

Left: Places the graphic at the left margin

Right: Places the graphic at the right margin

%< LeftHeaderGraphic <Filename> %>
%< CenterHeaderGraphic <Filename> %>
%< RightHeaderGraphic <Filename> %>
%< LeftFooterGraphic <Filename> %>
%< CenterFooterGraphic <Filename> %>

%< RightFooterGraphic <Filename> %>: These six commands specify the graphics to be used in the header and footer. The first two words of the command give the location of the graphic. The graphics take effect at the next header for the header commands and at the next footer for the footer commands. The same file formats as for the Graphic command above are supported. If these commands are not present, then the standard header and footer graphics as specified in options will be used. The header graphics are aligned so that the bottom edge of each graphic is aligned with the bottom of the header. The footer graphics are aligned so that the top edge of each graphic is aligned with the top of the footer. If both text and graphic headers and footers have been specified, then the text component will overwrite the graphic component.

Common Parameters for Plots and 3D Plots

Plots and 3D plots have a common set of parameters in addition to particular parameters for each kind of document. The instructions will include either the item Plot or the item Plot3D. When one of these appears in the instruction, the following items can be used to modify the appearance of the plot:

NoTitle: Removes the title from the plot

Width: Specifies the width in inches

Height: Specifies the height in inches

Center: Horizontally centers the plot

Left: Places the plot at the left margin

Right: Places the plot at the right margin

Common Parameters for Tables

Tables have a common set of parameters in addition to particular parameters for each kind of document. The instructions will generally include the item Table, but other items such as Layers in a Design instruction also produce tables that can be controlled by these common parameters. When this item appears in the instruction, the following items can be used to modify the appearance of the table:

MaxFontSize: This parameter specifies that the table should be adjusted to fit the page width The parameter following MaxFontSize must be a number that specifies the maximum font size that may be used.

MinFontSize: This parameter specifies that the table should be adjusted to fit the page width The parameter following MinFontSize must be a number that specifies the minimum font size that may be used. If the table needs a smaller font to be displayed on one page, then the table will be broken up and displayed on several pages.

Iteration Instructions

Many documents make use of several other documents. For example, a design typically uses several materials and a Stack typically uses several designs. The iteration instructions provide a means for printing information from the sub-documents. The

iteration loop begins with a %<ForEach… >% and ends with a %<Next…>% instruction. The report generator performs the instructions in the loop for each sub-document of the type named in the ForEach instruction. Each time the report generator begins an iteration, the next sub-document in the list will be the document whose contents will be printed.

The following iteration instructions are recognized:

%<ForEachMaterial%> … %<NextMaterial%>: Iterates over the materials used. Can be used in Designs, Stacks, vStacks, Machine Configurations and Reverse Engineers,

%<ForEachSubstrate%> … %<NextSubstrate%>: Iterates over the substrates used. Can be used in Stacks and Machine Configurations,

%<ForEachDesign%> …%<NextDesign%>: Iterates over the designs used. Can be used in Stacks, vStacks.

%<ForEachChip%> … %<NextChip%>: Iterates over the chips used in a Runsheet.

%<ForEachMeasurement%> … %<NextMeasurement%>: Iterates over the measured spectra in a Reverse Engineer.

%<ForEachScript *ScriptName EntryPoint*%> … %<NextScript *ScriptName EntryPoint*%>: Iterates over a range defined in a script. For each iteration, the EntryPoint is called in the script ScriptName. More information on using ForEachScript is in the Report Generator section of the Scripting Language Help.

For example, the template fragment

```
%<ForEachMaterial%>
%<Material Title%>
%<NextMaterial%>
```

in a design report template will print out a list of the materials used in the design.

The Targets Instruction

%<Targets *Parameter*%> prints the target tables.

This instruction is only available in Designs, Stacks, and vStacks. The parameters are:

Standard: Prints the standard targets

Color: Prints the color targets

Thickness: Prints the thickness targets (only for designs)

The common table parameters described above may also be used

Material Report Templates

Templates for materials can contain the page layout instructions described above and the material instruction used as many times as necessary to print the desired information about the material. The material instruction may also be used in a template for any file that uses materials, such as Design and Stack files, inside a %<ForEachMaterial%> … %<NextMaterial%> loop. The material instruction has the form:

%<Material *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot and how the plot and table are formatted.

Parameters

Plot: Prints a plot of the material
- **Wavelength**: Specifies that the plot will use a wavelength axis
- **Frequency**: Specifies that the plot will use a frequency axis
- The common plot parameters described above may also be used

Table: Prints the table of data
- The common table parameters described above may be used

Notes: Prints the notes

PoissonsRatio: Prints the value or “undefined”

LinearExpansionCoefficient: Prints the value or “undefined”

ThermalIndexCoefficient: Prints the value or “undefined”

YoungsModulus: Prints the value or “undefined”

ReferenceStress: Prints the value or “undefined”

ReferenceTemperature: Prints the value or “undefined”

SurfaceEnergy: Prints the value or “undefined”

Title: Prints the name of the material

Script: Runs the specified script and inserts the result into the report. See the Report Script section below for more information.

Substrate Report Templates

Templates for substrates can contain the page layout instructions described above and the substrate instruction used as many times as necessary to print the desired information about the substrate. The substrate instruction may also be used in a template for any file that uses substrates, such as Stack files, inside a %<ForEachSubstrate%> … %<NextSubstrate%> loop. The substrate instruction has the form:

%<Substrate *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot and how the plot and table are formatted.

Parameters

Plot: Prints a plot of the substrate
Wavelength: Specifies that the plot will use a wavelength axis
Frequency: Specifies that the plot will use a frequency axis
The common plot parameters described above may also be used

Table: Prints the table of data

The common table parameters described above may be used

Notes: Prints the notes

Thickness: Prints the thickness

ThicknessUnit: Prints the thickness units

Title: Prints the name of the substrate

Script: Runs the specified script and inserts the result into the report. See the Report Script section below for more information.

Design Report Templates

Templates for designs can contain the page layout instructions described above, the design instruction used as many times as necessary to print the desired information about the design. The design instruction may also be used in a template for any file that uses designs, such as Stack and vStack files, inside a %<ForEachDesign%> … %<NextDesign%> loop. The design instruction has the form:

%<Design *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot and how the plot and table are formatted.

To print out information about the targets, use the **Target** instruction described above.

A design template may also contain a %<ForEachMaterial%> … %<NextMaterial%> loop to print out information about the materials used in the design.

Parameters

Layers: Prints the layers in the design

Show: Forces the only columns named after the Show command to be displayed in the report regardless of whether they are displayed on the screen or not.

The following are the names of the columns for use with Show

MediumType
PackingDensity
RefractiveIndex
OpticalThickness
GeometricThickness
Locked
VoidMaterial
InhomogeneityFactor
MaximumPhysicalThickness
LayerNumber
Material
ExtinctionCoefficient
PhysicalThickness
MediumThickness
Link
VoidDensity
MinimumPhysicalThickness

For example

%<Design Layers Show LayerNumber Material PhysicalThickness %>

will cause only the layer number, material and physical thickness to be printed.

Plot: Prints a plot

Performance: Plots the performance of the design

Errors: Plots the variation in the performance given by the error parameters stored in the design

Admittance: Plots the admittance locus of the design

ReflectionCoefficient: Plots the reflection coefficient locus of the design

ElectricField: Plots the electric field of the design

AbsorptanceRate: Plots the absorptance rate of the design

TotalAbsorptance: Plots the total absorptance of the design

Color: Plots the color of the design

Errors: Plots the variation in color given by the error parameters stored in the design

Index: Plots the index profile of the design

The common plot parameters described above may also be used

Table: Prints a table

Performance: prints the performance table

Color: prints the color table

Admittance: Prints a table of admittance data

ReflectionCoefficient: Prints a table of reflection coefficient data

ElectricField: Prints the electric field data

AbsorptanceRate: Prints the absorptance rate data

TotalAbsorptance: prints the total absorptance data

The common table parameters described above may also be used

Plot3D: Prints the 3D plot of the design.

The common plot parameters described above may also be used

Notes: Prints the notes

IncidentAngle: Prints the incident angle

ReferenceWavelength: Prints the reference wavelength

IncidentAngleUnit: Prints the units of the incident angle

WavelengthUnit: Prints the units for wavelength

MatchAngle: Prints the match angle

MatchAngleKLimit: Prints the extinction coefficient limit used in Match Angle

Title: Prints the title of the file. This is the name of the file excluding the path and the extension.

Filename: Prints the complete filename of the design

Script: Runs the specified script and inserts the result into the report. See the Report Script section below for more information.

The following instructions can also be used in a design report template:

%<ForEachMaterial%>: Begins a loop iterating over each material used in the design

%<NextMaterial%>: Ends the loop iterating over each material

%<Material *Parameter*%>: Prints information about the current material as selected by ForEachMaterial.

For example:

```
%<ForEachMaterial%>
%<Material Title%>
%<Material Plot Wavelength NoTitle, Width 6 Height 4%>
%<NextMaterial%>
```

will print out the name and a plot of the material's optical constants for each material used in the Design

%<Targets *Parameter*%>: Prints information about the design's targets. The options for targets are defined above.

Stack Report Templates

Templates for stacks can contain the page layout instructions described above, the stack instruction used as many times as necessary to print the desired information about the stack. The stack instruction has the form:

%<Stack *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot or table and how the plot and table are formatted.

To print out information about the targets, use the **Target** instruction described above.

A stack template may contain a %<ForEachMaterial%> … %<NextMaterial%> loop to print out information about the materials used in the stack. This will include all the materials used in all the designs present in the stack. It may also contain a %<ForEachSubstrate%> … %<NextSubstrate%> loop to print out information about the substrates used in the stack. Information about the designs used in the stack are printed out using the %<ForEachDesign%> … %<NextDesign%> loop.

Parameters

Media: Prints the Stack table

Show: Forces the columns named after the Show command to be displayed in the report regardless of whether they are displayed on the screen or not.

The following are the names of the columns for use with Show

MediumType	**MediumMaterial**
MediumSubstrate	**MediumThickness**
CoatingFile	**CoatingDirection**
CoatlingLocked	

For example

%<Stack Media Show MediumMaterial MediumThickness CoatingFile %>

will cause the material, thickness and coating file columns to be printed. The other columns will not be printed.

The common table parameters described above may also be used

Plot: Prints the plot

Performance: Plots the performance of the stack

Errors: Plots the variation in the performance given by the error parameters

Color: Plots the color of the stack

Errors: Plots the variation in color given by the error

The common plot parameters described above may also be used

Plot3D: Prints the 3d plot

The common plot parameters described above may also be used

Table: Prints a table

Performance: Prints the performance table

Color: Prints the color table

The common table parameters described above may also be used

Notes: Prints the notes

Title: Prints the title of the file. This is the name of the file excluding the path and the extension.

Filename: Prints the complete filename of the stack

Script: Runs the specified script and inserts the result into the report. See the Report Script section below for more information.

The following instructions can also be used in a Stack report template:

%<ForEachMaterial%>: Begins a loop iterating over each material used in the stack

%<NextMaterial%>: Ends the loop iterating over each material

%<Material *Parameter*%>: Prints information about the current material as selected by ForEachMaterial. The options are as defined for materials above

%<ForEachSubstrate%>: Begins a loop iterating over each substrate used in the stack

%<NextSubstrate%>: Ends the loop iterating over each substrate

%<Substrate *Parameters*%>: Prints information about the current substrate as selected by ForEachSubstrate. The options are as defined for substrates above

%<ForEachDesign%>: Begins a loop iterating over each design used in the stack

%<NextDesign%>: Ends the loop iterating over each design

%<Design *Parameters*%>: Prints information about the current design as selected by ForEachDesign. The options are as defined for designs above

%<Targets *Parameters*%>: Prints information about the stack's targets. The options for targets are defined above.

vStack Report Templates

Templates for vstacks can contain the page layout instructions described above, the vstack instruction used as many times as necessary to print the desired information about the vstack. The vstack instruction has the form:

%<vStack *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot or table and how the plot and table are formatted.

To print out information about the targets, use the **Target** instruction described above.

A vstack template may contain a %<ForEachMaterial%> … %<NextMaterial%> loop to print out information about the materials used in the vstack. This will include all the materials used in all the designs present in the vstack. Information about the designs used in the vstack are printed out using the %<ForEachDesign%> … %<NextDesign%> loop.

Parameters

Media: Prints the vStack table

Show: Forces the columns named after the Show command to be displayed in the report regardless of whether they are displayed on the screen or not.

The following are the names of the columns for use with Show

FrontMaterial	**BackMaterial**
SurfaceAngle	**TransferMode**
CoatingFile	**CoatingDirection**
CoatingLocked	**ExitBeamAngle**
IncidentAngle	**EmergentAngle**

For example,

%<vStack Media Show FrontMaterial BackMaterial SurfaceAngle TransferMode CoatingFile IncidentAngle %>

will produce a six column table when printed in the report.

The common table parameters described above may also be used

Plot: Prints the plot

Performance: Plots the performance of the vstack

Errors: Plots the variation in the performance given by the error parameters

Color: Plots the color of the vstack

Errors: Plots the variation in color given by the error

The common plot parameters described above may also be used

Plot3D: Prints the 3d plot

The common plot parameters described above may be used

Table: Prints a table

Performance: Prints the performance table

Color: Prints the color table

The common table parameters described above may also be used

Notes: Prints the notes

Title: Prints the title of the file. This is the name of the file excluding the path and the extension.

Filename: Prints the complete filename of the vstack

Layout: Prints the vstack layout

Width: The next parameter specifies the width in inches

Height: The next parameter specifies the height in inches

The aspect ratio of the layout is kept the same as in the screen display. The layout is adjusted to fit the width and height specified.

The following instructions can also be used in a vStack report template:

%<ForEachMaterial%>: Begins a loop iterating over each material used in the vstack

%<NextMaterial%>: Ends the loop iterating over each material

%<Material *Parameter*%>: Prints information about the current material as selected by ForEachMaterial. The options are as defined for materials above

%<ForEachDesign%>: Begins a loop iterating over each design used in the vstack

%<NextDesign%>: Ends the loop iterating over each design

%<Design *Parameters*%>: Prints information about the current design as selected by ForEachDesign. The options are as defined for designs above

%<Targets *Parameters*%>: Prints information about the vstack's targets. The options for targets are defined above.

Machine Configuration Report Templates

Templates for machine configurations can contain the page layout instructions described above, the Machine instruction used as many times as necessary to print the desired information about the machine configuration. The machine instruction has the form:

%<Machine *Parameter*%>

where the parameter is selected from the list below. For tables, additional parameters may be added to control how the table is formatted.

A machine configuration template may contain a %<ForEachMaterial%> … %<NextMaterial%> loop to print out information about the materials used in the vstack. This will include all the materials used in all the designs present in the vstack. Information about the substrates used in the machine configuration are printed out using the %<ForEachSubstrate%> … %<NextSubstrate%> loop.

Parameters

Sources: Prints the sources table

The common table parameters described above may be used

Chips: Prints the chips table

The common table parameters described above may be used

CrystalToolingErrors: Prints the crystal tooling errors table

The common table parameters described above may be used

OpticalToolingErrors: Prints the optical tooling errors table

The common table parameters described above may be used

PackingDensityErrors: Prints the packing density errors table

The common table parameters described above may be used

DepositionRateVariation: Prints the deposition rate variation table

The common table parameters described above may be used

Notes: Prints the notes

Monitoring: Prints the monitoring type

IncidentAngle: Prints the incident angle

IncidentAngleUnit: Prints the units for the incident angle

DepositionMedium: Prints the deposition medium

ThicknessScaleFactor: Prints the thickness scale factor

ThicknessUnits: Prints the units for thickness

ResetToolingFactor: Prints the reset option, either "Yes" or "No" will be printed

GratingCalibrationFactor: Prints the grating calibration factor

Title: Prints the title of the file. This is the name of the file excluding the path and the extension.

Filename: Prints the complete filename of the machine configuration

Script: Runs the specified script and inserts the result into the report. See the Report Script section below for more information.

The following instructions can also be used in a Machine Configuration report template:

%<ForEachMaterial%>: Begins a loop iterating over each material used in the machine configuration

%<NextMaterial%>: Ends the loop iterating over each material

%<Material *Parameter*%>: Prints information about the current material as selected by ForEachMaterial. The options are as defined for materials above

%<ForEachSubstrate%>: Begins a loop iterating over each substrate used in the machine configuration.

%<NextSubstrate%>: Ends the loop iterating over each substrate

%<Substrate *Parameters*%>: Prints information about the current substrate as selected

by ForEachSubstrate. The options are as defined for substrates above

Runsheet Report Templates

Templates for runsheets can contain the page layout instructions described above, the Runsheet instruction used as many times as necessary to print the desired information about the runsheet. The runsheet instruction has the form:

%<Runsheet *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot and how the plot and table are formatted.

A runsheet template may also contain a %<ForEachChip%> … %<NextChip%> loop to print out signal plots for each different chip used in the runsheet.

Parameters

Plot: Plots the runsheet signal

Wideband: Generates the wideband plot

Narrowband: Generates the single wavelength plot

Chip: Generates the plot for the chip selected by ForEachChip below

AllChips: Generates the plot for all chips

The common plot parameters described above may also be used

Table: Prints the runsheet table

Show: Forces the columns named after the Show command to be displayed in the report regardless of whether they are displayed on the screen or not.

The following are the names of the columns for use with Show

Chip	**LayerNumber**
Source	**Material**
Thickness	**Wavelength**
Bandwidth	**ChipOpticalThickness**
MonitorSpectrum	**SimulationSpectrum**
ZeroOffset	**Gain**
MonitorType	**InitialSignal**
StartAt	**FirstMaxima**
FirstMinima	**LastMaxima**
LastMinima	**FinishAt**
FinalSwing	**Peaks**
NumberOfPeaks	**InitialDirection**
DesignRefractiveIndex	**DesignPhysicalThickness**

For example

%<Runsheet Table Show Chip Source Wavelength StartAt Peaks %>

will print out a five column runsheet

The common table parameters described above may also be used

Notes: Prints the notes

Design: Prints the filename of the design used

Machine: Prints the filename of the machine configuration used

Polarization: Prints the polarization of the optical signal

MonitorMode: Prints the monitor mode (Transmittance, Reflectance, Back Reflectance)

WavelengthInterval: Prints the wavelength interval used for the calculations

WavelengthScaleFactor: Prints the wavelength scale factor

UsePreviousExtremum: Prints the use previous extremum option, either "Yes" or "No" is printed

OneWavelengthPerChip: Prints the one wavelength per chip options, either "Yes" or "No" is printed

Title: Prints the title of the file. This is the name of the file excluding the path and the extension.

Filename: Prints the complete filename of the machine configuration

Script: Runs the specified script and inserts the result into the report. See the Report Script section below for more information.

The following instructions can also be used in a Runsheet report template:

%<ForEachChip%>: Begins a loop iterating over each chip used in the runsheet
%<NextChip%>: Ends the loop iterating over each chip

For example:

```
%<ForEachChip%>
%<Runsheet Plot Narrowband Chip%>
%<NextChip%>
```

will produce a separate plot for each chip in the runsheet.

%<Design *Parameter*%>: Prints design information for the design used in the runsheet

%<Machine *Parameter*%>: Prints machine configuration information for the machine configuration used in the runsheet

Optical Constant Report Templates

Templates for optical constants can contain the page layout instructions described above, the OpticalConstant instruction used as many times as necessary to print the desired information. The OpticalConstant instruction has the form:

%<OpticalConstant *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot and how the plot and table are formatted.

Parameters

Plot: Prints a plot

- **Transmittance**: Prints the transmittance plot
- **Reflectance**: Prints the reflectance plot
- **SubstrateTransmittance**: Prints the substrate transmittance plot
- **SubstrateReflectance**: Prints the substrate reflectance plot
- **OpticalConstants**: Prints the optical constants plot
- The common plot parameters described above may also be used

Table: Prints a table

- **Data**: Prints the extrema data points
- **OpticalConstants**: Prints the optical constant data
- The common table parameters described above may also be used

Notes: Prints the notes

FilmThickness: Prints the film thickness

ApproximateIndex: Prints the approximate film thickness

Tolerance: Prints the R/T tolerance

IncidentAngle: Prints the incident angle

IncidentAngleUnit: Prints the units of incident angle

Polarization: Prints the polarization of the measuring light

SingleSidedReflectance: Prints the single sided reflectance option, either “Yes” or “No” is printed

UseSpectrum: Prints the use spectrum option, either “Yes” or “No” is printed

SmoothData: Prints the smooth data option, either “Yes” or “No” is printed

SubstrateThickness: Prints the thickness of the substrate

SubstrateThicknessUnit: Prints the units for the substrate thickness

Title: Prints the title of the file. This is the name of the file excluding the path and the

extension.

Filename: Prints the complete filename.

The following instructions can also be used in a Optical Constant report template:

%<SubstrateSubstrate *Parameter*%>: Prints Substrate data for the substrate used. Options are defined in substrate above

%<SubstrateMaterial *Parameter*%>: Prints Material data for the material used in the substrate. Options are defined in material above

Reverse Engineer Report Templates

Templates for reverse engineering can contain the page layout instructions described above, the Reverse Engineer instruction used as many times as necessary to print the desired information. The Reverse Engineer instruction has the form:

%<ReverseEngineer *Parameter*%>

where the parameter is selected from the list below. For plots and tables, additional parameters may be added to control the kind of plot and how the plot and table are formatted.

Parameters

Plot: Prints a plot

Measurement: Plots the current measurement plot. The current plot is controlled by the ForEachMeasurement loop

SystematicThickness: plots the systematic thickness variation of the adjustment

SystematicPackingDensity: plots the systematic packing density variation of the adjustment

SystematicInhomogeneity: plots the systematic inhomogeneity variation of the adjustment

RandomThickness: plots the random and systematic thickness variation of the adjustment

RandomPackingDensity: plots the random and systematic packing density variation of the adjustment

RandomInhomogeneity: plots the random and systematic inhomogeneity variation of the adjustment

Spectra: plots the variation in the measurements used in the adjustment

The common plot parameters described above may also be used

Table: Prints the design and adjustment table

Show: Forces the only columns named after the Show command to be displayed in the report regardless of whether they are displayed on the screen or not.

The following are the names of the columns for use with Show

LayerNumber
Material
ExtinctionCoefficient
PhysicalThickness
Locked
VoidMaterial
InhomogeneityFactor
MaximumPhysicalThickness
MaximumOpticalThickness
SystematicPackingDensity
RandomThickness
RandomInhomogeneity
PackingDensity
RefractiveIndex
OpticalThickness
GeometricThickness
Link
VoidDensity
MinimumPhysicalThickness
MinimumOpticalThickness
SystematicThickness
SystematicInhomogeneity
RandomPackingDensity

For example

```
%<ReverseEngineer Table Show LayerNumber SystematicThickness
RandomThickness %>
```

will cause only the layer number, systematic thickness changes and random thickness changes to be printed.

The common table parameters described above may also be used

RMSDifference: Prints the RMS Difference

MediumMaterial: Prints the name of the medium material

SubstrateMaterial: Prints the name of the substrate material

SubstrateBulk: Prints the name of the substrate internal transmittance data

SubstrateType: Prints whether the calculations are performed using a parallel substrate (“Parallel”) or a wedged substrate (“Wedged”).

SubstrateThickness: Prints the thickness of the substrate.

SubstrateThicknessUnit: Prints the units of substrate thickness

IncidentAngle: Prints the incident angle

IncidentAngleUnit: Prints the incident angle units

Polarization: Prints the polarization state of the measurement.

MagnitudeType: Prints the type of measurement (“Transmittance” or “Reflectance”)

Title: Prints the title of the file. This is the name of the file excluding the path and the extension.

Filename: Prints the complete filename.

The following instructions can also be used in a Optical Constant report template:

%<SubstrateBulk *Parameter*%>: Prints Substrate data for the substrate used. Options are defined in substrate above

%<SubstrateMaterial *Parameter*%>: Prints Material data for the material used in the substrate. Options are defined in material above

%<MediumMaterial *Parameter*%>: Prints Material data for the material used as the medium. Options are defined in material above

%<Material *Parameter*%>: Prints Material data for the current material in the ForEachMaterial loop. Options are defined in material above

%<ForEachMaterial%>: Begins a loop iterating over each material used in the Reverse Engineer

%<NextMaterial%>: Ends the loop iterating over each material

%<ForEachMeasurement%>: Begins a loop iterating over each measurement in the Reverse Engineer

%<NextMeasurement%>: Ends the loop iterating over each measurement

Report Scripts

If you have the Function Enhancement, you can, for supported files, write scripts to create plots, tables and text to be included in a report. The report template can contain an instruction to call a script and put the result of that script into the report. The general syntax of the instruction is:

%<*FileType* Script *ScriptName EntryPoint ReturnType Parameters*%>

The *FileType* names the type of the data file that script will be using. It is one of Material, Substrate, Design, Stack, MachineConfiguration, Runsheet. *ScriptName* is the filename containing the script. *EntryPoint* is the name of the function to call in the script. *ReturnType* is the type of data that will be returned by *EntryPoint*. *ReturnType* is one of Plot, Table, String. *Parameters* are any parameters appropriate to the *ReturnType*. If the *ReturnType* is Plot, then appropriate parameters are any of the common parameters for plots (see above). If the *ReturnType* is Table, then appropriate parameters are any of the common parameters for tables (see above). When the *ReturnType* is String, there are no parameters.

When a *ScriptName* appears for the first time in a report template, the subroutine InitializeReport in the script will be called. This subroutine does not have to be defined, but if it is defined, its instructions will be performed. These can include performing

common calculations, collecting parameters from the user via a dialog, setting up data etc.

For an *EntryPoint* with a *ReturnType* of Plot, the entry point must be defined as a function:

```
Function EntryPointName As Object
```

The function must return a PlotCreator object e.g.

```
Set EntryPointName = myPlotCreator
```

For an *EntryPoint* with a *ReturnType* of Table, the entry point must be defined as a function:

```
Function EntryPoint As Object
```

The function must return a Table object e.g.

```
Set EntryPointName = myTable
```

For an *EntryPoint* with a *ReturnType* of String, the entry point must be defined as a function:

```
Function EntryPointName As String
```

The function must return a string e.g.

```
EntryPointName = "Hello World"
```

For more information on scripts and the objects referenced here, please see the Scripting Help section of the online Help available in the Help menu of the Essential Macleod.

Some Examples

Design Report Template

This is a simple template that will show the performance of the design followed by its structure.

The report template is:

```
%<Portrait%>
%<Font Size 18 Bold Name Arial%>
%<Design Title%>
%<Font Size 12 NoBold Name "Times New Roman"%>
This design is stored in %<Design Filename%>

%<Design Plot Performance NoTitle Width 6 Height 4%>
```

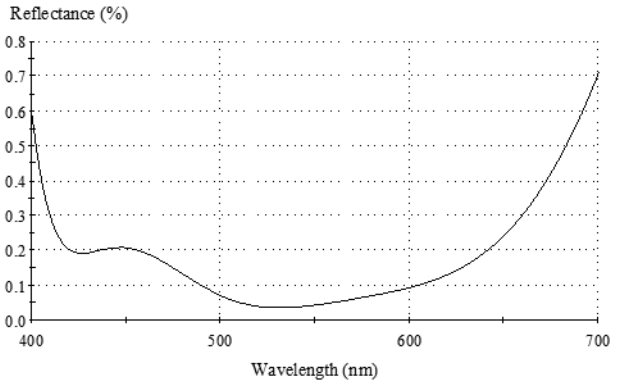
%<Design Layers%>

Sample Output

Design: Four Layer AR

Four Layer AR

This design is stored in C:\Program Files\Thin Film Center\Designs\Four Layer AR.dds



Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
Medium	Air	1.00000	0.00000		
1	MgF2	1.38455	0.00000	0.25169940	92.71
2	ZrO2	2.06576	0.00004	0.53354450	131.72
3	MgF2	1.38455	0.00000	0.08233427	30.33
4	ZrO2	2.06576	0.00004	0.06699026	16.54
Substrate	Glass	1.52077	0.00000		
				0.93456843	271.30

Runsheet Report Template

%<Landscape%>
%<Font Size 18 Bold %>
%<Runsheet Title%>
%<Font Size 8.25 NoBold %>
This Runsheet is stored in %<Runsheet Filename%>

%<Runsheet Table MinFontSize 4 %>

%<Runsheet Plot NoTitle NarrowBand AllChips Width 6 Height 4%>
%<NewPage%>
%<Design Title%>
%<Design Plot Performance NoTitle Width 6 Height 4%>

%<Design Layers%>

Sample Output

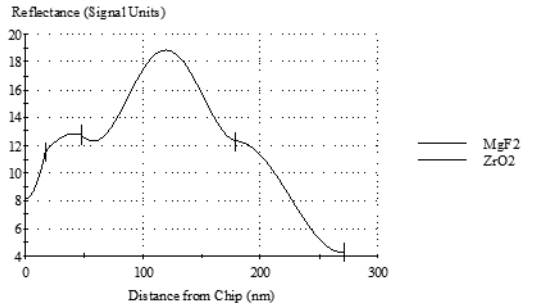
This template results in a multi-page output:

Runsheet: 4 Layer AR

4 Layer AR

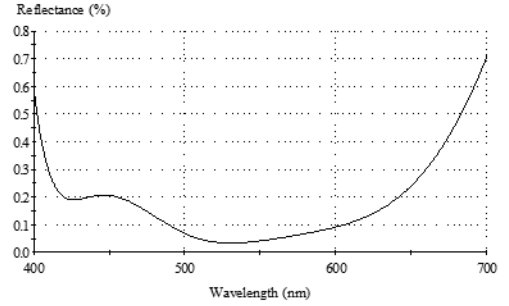
This Runsheet is stored in C:\Program Files\Thin Film Center\Designs\4 Layer AR.rs

Chip	Layer	Source	Monitor Wavelength (nm)	Monitor Bandwidth (nm)	Start At	First Maxima	First Minima	Last Maxima	Last Minima	Finish At	Final Swing	Peaks
1: Glass	1	ZrO2	510.00	10.00	8.1866					11.5236	40.7617	↑↓
	2	MgF2	510.00	10.00	11.5236	12.8535				12.7827	5.3282	↑
	3	ZrO2	510.00	10.00	12.7827	18.8621	12.3004			12.3202	99.6985	↓↑
	4	MgF2	510.00	10.00	12.3202		4.3049			4.3141	0.1143	↓



Runsheet: 4 Layer AR

Four Layer AR



Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
Medium	Air	1.00000	0.00000		
1	MgF2	1.38455	0.00000	0.25169940	92.71
2	ZrO2	2.06576	0.00004	0.53354450	131.72
3	MgF2	1.38455	0.00000	0.08233427	30.33
4	ZrO2	2.06576	0.00004	0.06699026	16.54
Substrate	Glass	1.52077	0.00000		
				0.93456843	271.30

vSTACK

vStack is the tool that calculates the properties of assemblies of coatings and substrates where the substrates are not necessarily parallel-sided. The system of elements is known as a vStack and it consists of a series of *Surfaces*. Each surface may be uncoated or it may carry one optical coating. When there is only one surface then the system will appear exactly as a single coating on an infinite substrate but usually there will be a number of surfaces with associated coatings. vStack assumes that all beam directions and surface normals are coplanar.

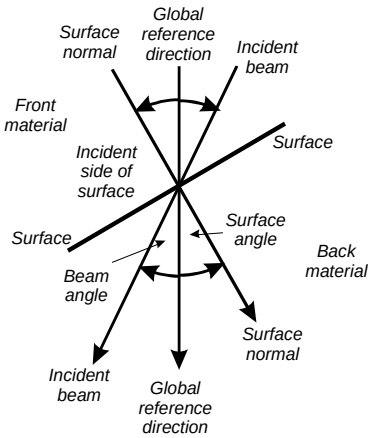
The calculations performed by vStack apply to the path of a single beam through the assembly. This is in contrast to the Stack system where multiple reflections may be taken into account. The path of the beam is defined by the list of surfaces. The terms incident and emergent can be confusing since the surfaces may operate in transmission or reflection and the beams may not emerge in what has been called the emergent medium. We therefore use the terms *front material* and *back material* to refer to the two media on either side of each surface. The light is incident in the front material.

The *transfer mode* of a surface defines how the beam it is treated at the surface. There are eight transfer modes*: Transmit, Reflect, Perfect Reflect, Rotate 0, Rotate 90, Rotate 180, Rotate –90, and Perfect Retro*. Transmit and Reflect both calculate the effect of the front and back surfaces and the coating (f any) on the beam. For a surface that has transfer mode equal to *Transmit* the transmitted beam is taken and the reflected beam is discarded. The transmitted beam exits the surface in the back material. For a surface that has transfer mode equal to *Reflect*, the reflected beam is taken and the transmitted beam is discarded. The reflected beam exits the surface in the front material. The exit material for the beam depends on the transfer mode. The *Perfect Reflect* transfer mode behaves as a perfect reflector – 100% of the incident beam is reflected. Perfect Reflect does not require any front/back material definitions - the definitions from the surrounding surfaces are used. The *Perfect Retro* transfer mode behaves as a perfect retro-reflector – 100% of the incident beam is reflected back along the same path on which the beam entered the retro-reflector.. Perfect Retro does not require any front/back material definitions - the definitions from the surrounding surfaces are used.

The *Rotate* transfer modes rotate the beam about its axis. The convention for the rotation is that looking along the direction of the beam a positive rotation is counter-clockwise. *Rotate 0* has no effect on the beam and is included to make easy to turn beam rotation off without removing a surface. *Rotate 90* rotates the beam 90 degrees counter-clockwise. The output p-polarization component is the input s-polarization component. The output s-polarization component is the negative of the input p-polarization component. *Rotate 180* rotates the beam 180 degrees. The output p-polarization component is the negative of the input p-polarization component. The output s-polarization component is the negative of the input s-polarization component. *Rotate –90* rotates the beam 270 degrees (or 90 degrees clockwise). The output p-polarization component is the negative of the input s-polarization component. The output s-polarization component is the input p-polarization component. The *Rotate* transfer modes do not require any front/back material definitions – the definitions from the surrounding surfaces are used.

The light enters the assembly in the front material of the first surface in the list. The beam exits the assembly through either the front or back material of the last surface depending upon the transfer mode of the last surface.

As substrates are now not necessarily parallel-sided, there has to be a method of specifying the angular relationship between surfaces and the various beam directions. We therefore set up a *global reference direction* that does not vary throughout the entire system. All directions are then specified with respect to this reference direction.



This figure shows the various directions associated with a single surface. First of all we have a global reference direction that applies to the entire system and does not change from one surface to another. Each individual surface has a surface normal directed into the surface from the front material and out of the surface into the back material, following the same convention as the *z*-axis for a coating on a single surface. Finally there is the direction of the incident beam. The *surface angle* specifies the angle that the surface normal makes with the reference direction. Imagine that the surface normal is first placed in coincidence with the reference direction so that the directions are identical. Now let the surface normal be rotated into its correct orientation. The angle of rotation is the surface angle. It is positive if the rotation is counterclockwise and negative if clockwise - the normal sign convention for angles. The *beam angle* is determined similarly. The beam is imagined coincident with the reference direction and then is rotated to the correct position. The angle of rotation, following the same sign convention, is the beam angle. In the diagram the surface angle shown is positive and the beam angle negative.

With the reference direction constant, this procedure is then repeated for each subsequent surface in the vStack.

Note that the user need specify a beam angle only for the original direction of the light in the front material in the first surface of the vStack. This material is the incident medium for the entire system. The program takes care of all subsequent beam angles. An output parameter calculated and presented by the program is the beam angle in the final output medium.

vStack can operate with either a distance between surfaces specified in the Beam Distance column or with an unspecified distance between surfaces (Beam Distance left blank). When a Beam Distance is specified, the distance is from the surface on the

current row to the surface on the next row in the direction of the beam. Where the distance between surfaces is unspecified, vStack does not take into account any absorption in material between the surfaces. Where the distance between surfaces is specified, vStack will calculate the absorption in the material and include it in the performance results. It uses the real refractive indices at the appropriate wavelength and Snell's Law to calculate the beam direction. For unspecified Beam Distances, vStack also assumes that the path of the beam is geometrically valid – that is the path of the beam described is the actual path taken for the range of input beam angles used. Where Beam Distances have been specified, vStack will check for geometric validity. A graphical tool, described later, is supplied to help the user verify the specification of the vStack.

Absorption in a coating is included in the calculations using the extinction coefficients of the films in the normal way, and any extinction coefficient of the back material will be automatically included when calculating the performance of the coatings. Thus an internally reflecting prism surface that is coated with opaque aluminum will be correctly modeled if the surface is considered uncoated with a back material of aluminum and a transfer mode of "Reflect." It will not be correctly modeled if the transfer mode is changed to "Transmit." In that case the aluminum will need to be included in the surface coating and the back material changed to "Air."

A coated surface is specified by giving the filename of a coating and providing a coating direction. Coating direction may be either forward or reverse. A forward coating direction specifies that the layer next to the medium in the design is next to the front material of the surface. A reverse direction specifies that the layer next to the medium in the design is next to the back material of the surface. For refinement control a coating may also be specified as locked. This prevents refinement from altering the coating.

A vStack system may contain both reflecting and transmitting elements. Also there is only a single path through the system. This means the performance terms Transmittance and Reflectance become confusing, so vStack calculates Throughput which is defined as the ratio of the intensity of the beam exiting the vStack system to the intensity of the beam entering the vStack system. vStack also calculates the ellipsometric parameters for the system, Psi and Delta.

While the beam is confined to the plane of the instrument there is no mixing of the initially p- and s-polarized light. Each could be followed through the system completely separately. For *Transmit*, *Reflect* and *Perfect Reflect* surfaces, all p-polarized light entering the surface leaves the surface p-polarized and all s-polarized light entering the surface leaves the surface p-polarized. For rotator surfaces, all p-polarized light is converted into s-polarized light (for 90 and –90) and all s-polarized light is converted in to p-polarized light (for 90 and –90) When the beam direction is tilted out of the plane of the instrument this is no longer true. The plane of incidence is then rotated with respect to the plane of the instrument and there is now a mixing of the two principal polarizations. Some light that was originally s-polarized emerges finally from the system as p-polarized and some p-polarized light becomes s-polarized. We call this polarization leakage. The angle of tilt of the beam out of the plane of the instrument we call the skew angle and the sense is such that the rotation vector for a positive angle is along the positive p-direction. For a small skew angle the magnitude of the leakage is proportional to the square of the skew angle and so we define a polarization leakage coefficient with units of magnitude per unit skew angle^2, for example %/deg^2. The leakage coefficients can be either from p-

to s-polarization or vice versa. These coefficients are not necessarily equal. There is a constant phase relationship between the orthogonally polarized primary and leakage light and so we define also an appropriate Delta value. VStack will also calculate the total phase change contribution of all the coatings in the model. This does not include any phase effects caused by the substrates. Although this phase calculation is incomplete for the modeled system, it does provide information about the contribution of the coatings to wavefront distortion.

The complete set of parameters is then:

Throughput
Psi
Delta
p-s Leakage Coefficient
s-p Leakage Coefficient
p-s Delta
s-p Delta
Phase

Psi is defined as:

$$\arctan\left(\frac{\sqrt{p-throughput\ magnitude}}{\sqrt{s-throughput\ magnitude}}\right)$$

Delta is defined as:

$$(p-throughput\ phase) - (s-throughtput\ phase)$$

For reflecting surfaces, the ellipsometric convention is used. That is, at normal incidence, the Delta of a reflecting surface is 180 degrees. The absolute phase of the throughput polarizations is not available.

p-s Leakage is the proportion, for unit skew angle, of light exiting the vStack with s-polarization that entered the vStack with p-polarization.

s-p Leakage is the proportion, for unit skew angle, of light exiting the vStack with s-polarization that entered the vStack with s-polarization.

p-s Delta is defined as:

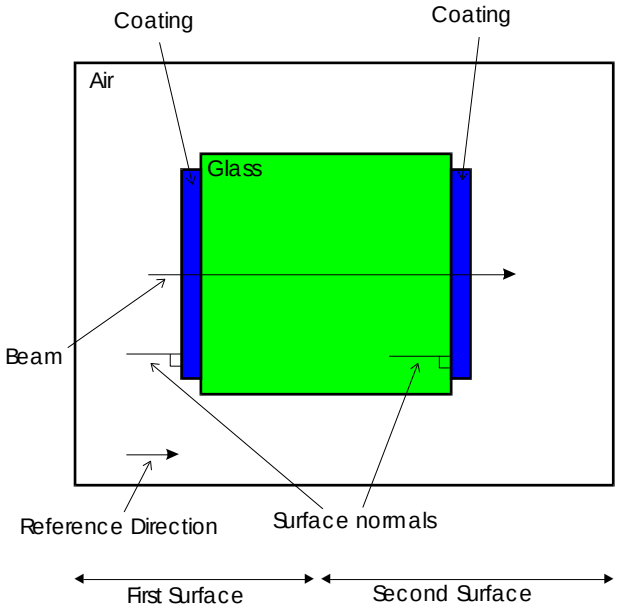
$$(p-throughput\ phase) - (p-s\ leakage\ phase)$$

s-p Delta is defined as:

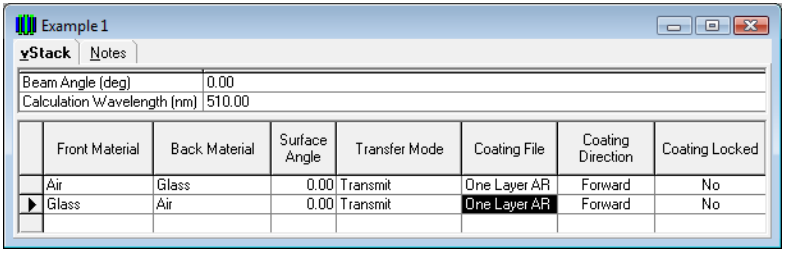
$$(s-p\ leakage\ phase) - (s\ throughput\ phase)$$

Example 1: A Single Substrate Coated Both Sides

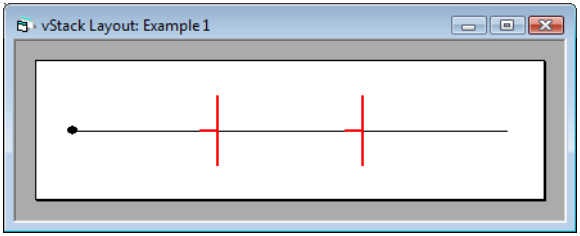
This example models a parallel sided glass substrate that has been coated on both sides with a 1 layer anti-reflection coating. This system can also be modeled by Stack for comparison of result. When modeling with Stack, be sure to set the medium to wedged to eliminate multiple reflections.



In vStack, this system is modeled with two surfaces. The first surface represents the beam entering the glass substrate through the coating and the second surface represents the beam exiting the glass though the second coating. The diagram above also shows the chosen reference direction for specifying the surface angles and the beam angle. The vStack shown below models this system.

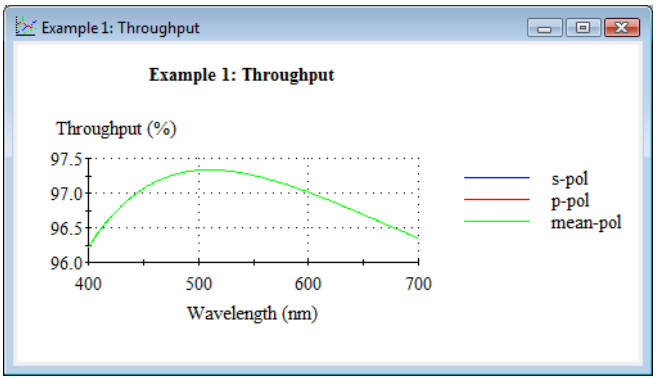


The first line of Example 1 represents the first interface that the beam passes through. The beam is initially in the front material – Air, then passes through the coating “one layer ar.dds” and then into the back material – Glass. The second line represents the second interface that the beam passes through. This time the front material is Glass. This is the material that already contains the beam from the first surface and so should match the back material of the first surface. On transition through the interface, the beam exits in Air. The coating on the second surface has a direction of reverse because the layer next to the medium in the design “one layer ar.dds” should be next to the Air. Click Draw Layout in the Tools menu and the following layout is drawn.

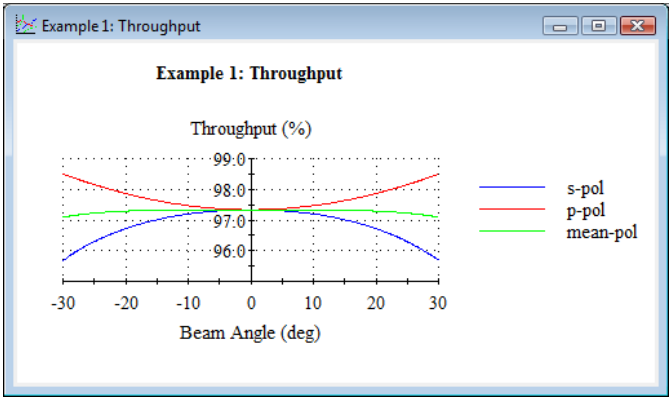


The black circle indicates the starting point of the light beam. The red lines show the interfaces. The small red line perpendicular to the large red line defines the front side of the interface. Solid black lines indicate unspecified beam distances and dashed black lines indicate specified beam distances. The lengths in the diagram will be proportional to the actual beam distances.

The throughput of this system is shown below.

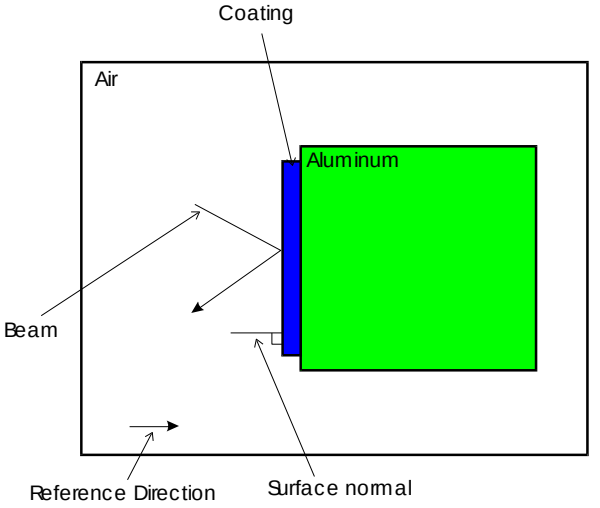


For a beam angle of zero, there is no polarization sensitivity and all curves follow the same path. The next plot shows the throughput of the system at 510 nm as the beam angle is varied from –30 to +30 degrees. As the surfaces of the system are parallel, there is no difference in performance between positive and negative beam angles.

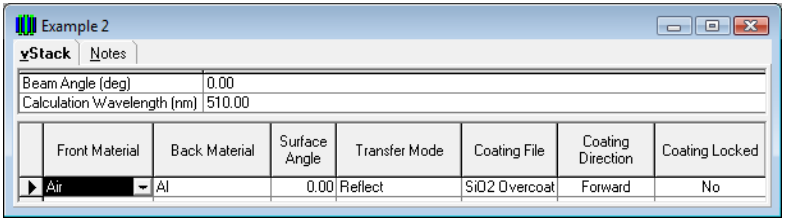


Example 2: A Single Reflecting Substrate

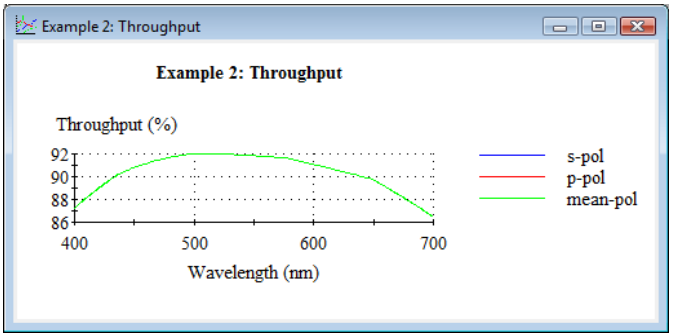
This example models a single reflecting surface. This system can also be modeled by the design editor for comparison of results.



In this case, we are only interested in the reflected signal from the first surface, so only one surface is needed to model this system.



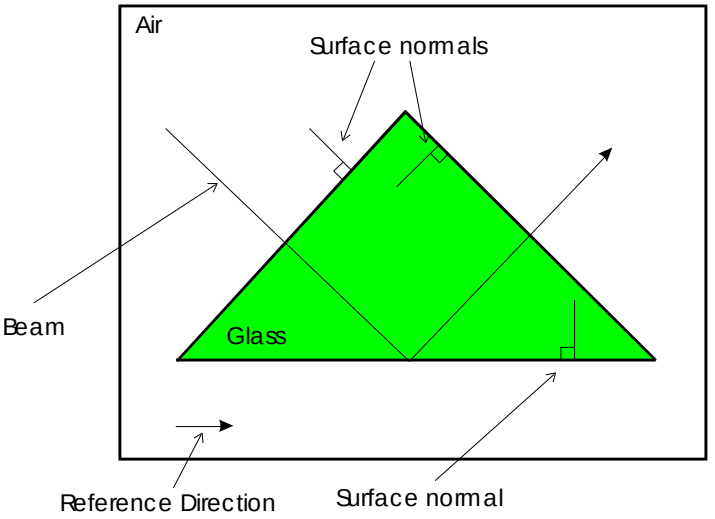
The curve below shows the performance of this overcoated aluminum reflector.



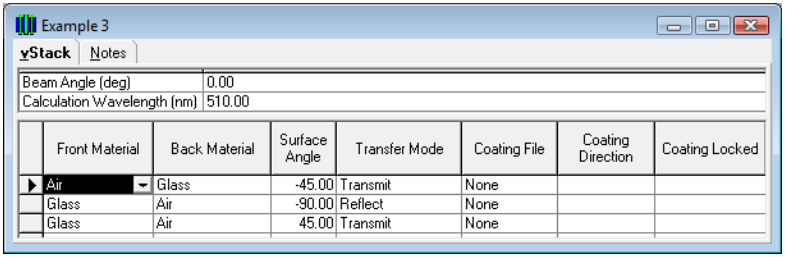
In this case, the throughput is describing the reflection performance of the system at normal incidence.

Example 3: Total Internal Reflection in an Uncoated Prism

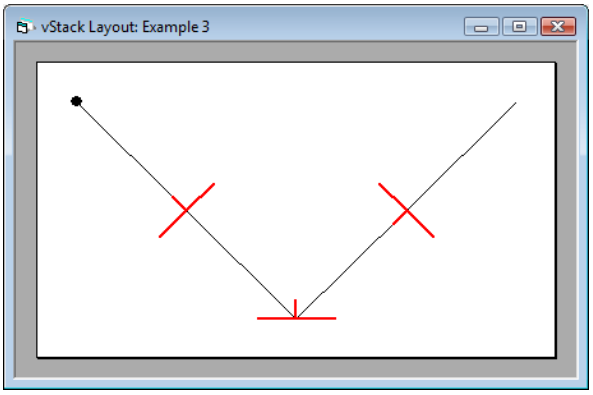
This example calculates the single beam performance of a right-angle prism. The layout is shown below.



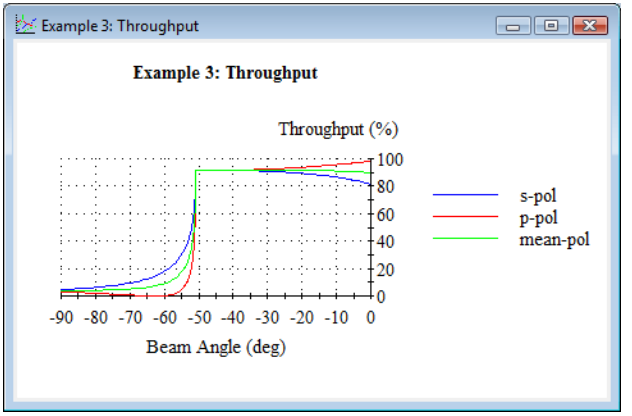
This is modeled as shown below.



If the beam is to enter the prism normal to the first surface, then the beam angle must be set to the same value as the surface angle - -45 degrees (or 315 degrees). The throughput of this system is the same as the throughput through a parallel-sided sheet of glass. Using the Draw Layout command with a Beam Angle of –45 gives the following diagram.



A more interesting case is to examine the throughput as the beam angle is varied. The plot below shows the variation of throughput as the beam is varied +/-45 degrees about the normal to the first surface. This corresponds to a beam angle range of –90 to 0 degrees, with –90 representing a beam flowing vertically down through the first interface and 0 representing a horizontal beam flowing into the first interface. The plot shows the throughput of the initial beam angles (starting at –90) at very low values. This happens because the beam strikes the second surface below the critical angle and so most of the energy is actually transmitted through the interface and only a small quantity is reflected. As the beam angle increases, the angle of the beam striking the second surface moves beyond the critical angle, and the second surface reflects the beam.



As the beam angle increases still further, the second surface still provides total internal reflection, but the increasing incident angle at the first and third surfaces causes the s- and p-polarizations to deviate from the mean throughput.

Note that the beam always passes through the three surfaces in the model whereas in a real system it may not. For example if the beam always entered the prism at the point shown in the layout diagram above, a beam with angle –90 degrees would enter the prism and the reflected energy would actually exit through the first surface and not the third. The throughput of this beam can be modeled by setting the surface angle of the third surface to be 135 degrees (180 degrees away from the first surface because the beam is travelling from glass to air)

Refinement and Synthesis

Refinement options are described in detail in the Refinement and Synthesis chapter of this manual. For vStack refinement, however, there are some additional conventions that are described here.

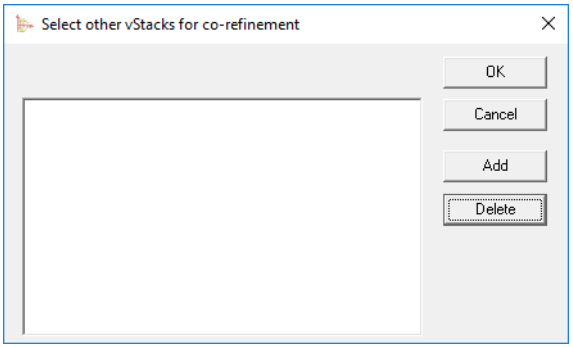
The refinement menu is found under **Parameters**. **Tools** exist for entering targets, adjusting refinement parameters and performing refinement. These menus are similar to those provided for refinement of single coatings. The **Coating Locked** column in the vStack window specifies that a particular coating in the vStack will not take part in the refinement. Only coatings with a **Coating Locked** value of **No** will take part in refinement.

Coatings are implicitly linked by name in a vStack. If the same coating design file is used on more than one surface in a vStack, then refinement will adjust a single copy of the design and apply it to all surfaces using the same design name. If you want to allow refinement to treat all coating designs separately, but want to have the same starting point, then the design must be copied to new files, one for each surface that is to have the same starting point.

vStacks additionally support Co-Refinement. Co-Refinement is the capability of simultaneous refinement of more than one vStack. A vStack models the path of a single beam through a system. If a beamsplitter is being modeled, then two vStacks are required. One vStack will model the transmitted path and the other will model the

reflected path. Without co-refinement, the beamsplitter coating cannot be refined in a single vStack because only the transmitted beam or the reflected beam can be defined. With co-refinement the filename of the transmitted beam model is given in the reflected beam vStack. Whenever the reflected beam vStack is refined, the transmitted beam vStack will also be refined. Co-refined vStacks are only loaded from the main vStack. If a vStack in the co-refinement list also has vStacks listed in its co-refinement list, these vStacks will NOT be co-refined.

The co-refinement list is displayed and edited by clicking **Co-refinement** in the **Refinement** sub-menu of the **Parameters** menu of the vStack. The following dialog is displayed:

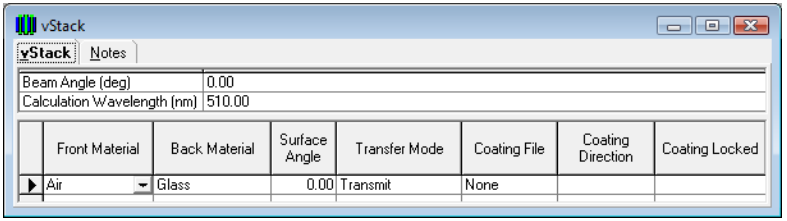


To add a vStack to the list, click **Add**. A file chooser will be displayed. Select the file to be added and click **Open**. To remove a file from the list, select the file in the list and click **Delete**. Clicking **OK** will update the vStack with the changes. Clicking **Cancel** will close the dialog and discard any changes.

vStack Menu

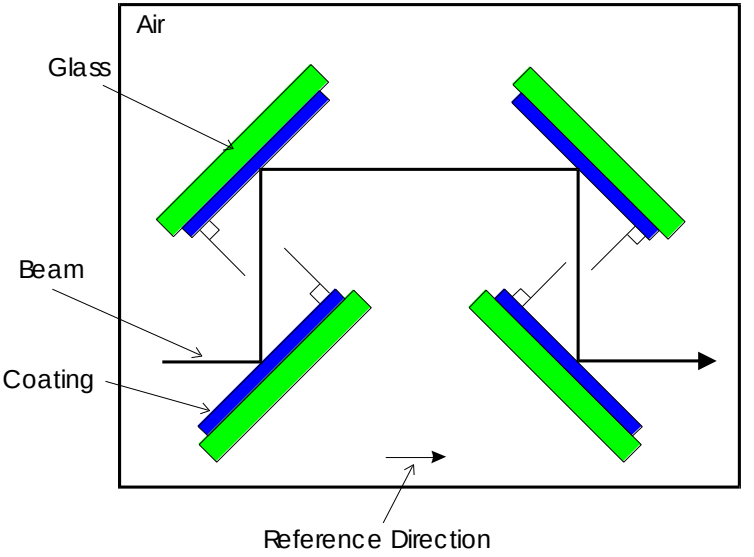
This menu is obtained when the vStack window is active. We illustrate its use with an example.

If in the **New...** dialog box from the **File** menu we select **vStack** and click **OK** it brings up a new vStack window. It may be necessary to drag the right-hand boundary to reveal all of the columns.



The first four columns apply to the media of the vStack. The final three columns are concerned with the coatings. Since this is a new vStack, it is very simple and consists of a

single interface. There are no coatings. We will construct the chevron filter that is developed in the Function chapter, but we will use vStack to calculate its properties. An 11-layer Zr02/SiO2 quarterwave multilayer at a reference wavelength of 300nm and a match angle of 45 degrees is used to provide the basic reflector. This filter is used on the four surfaces of the filter as shown below



We first create the reflector coating as below:

Design3

Design | Context | Notes

Incident Angle (deg)	0.00
Reference Wavelength (nm)	300.00

	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
▶	Medium	Air	1.00000	0.00000		
	1	ZrO2	2.15300	0.00216	0.26607307	37.07
	2	SiO2	1.48780	0.00000	0.28564202	57.60
	3	ZrO2	2.15300	0.00216	0.26607307	37.07
	4	SiO2	1.48780	0.00000	0.28564202	57.60
	5	ZrO2	2.15300	0.00216	0.26607307	37.07
	6	SiO2	1.48780	0.00000	0.28564202	57.60
	7	ZrO2	2.15300	0.00216	0.26607307	37.07
	8	SiO2	1.48780	0.00000	0.28564202	57.60
	9	ZrO2	2.15300	0.00216	0.26607307	37.07
	10	SiO2	1.48780	0.00000	0.28564202	57.60
	11	ZrO2	2.15300	0.00216	0.26607307	37.07
	Substrate	Glass	1.55277	0.00001		
					3.02464852	510.43

This coating is then saved in the file “chevron coating”.

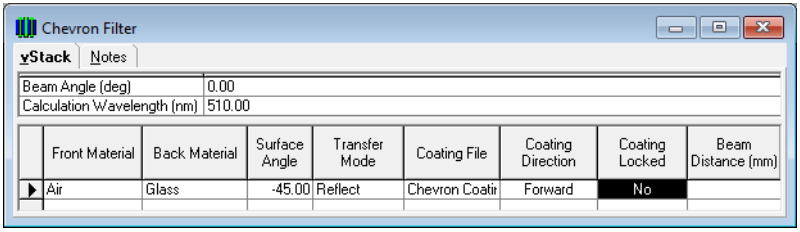
In vStack we will now create the four surfaces and apply the coating to the four surfaces. Click the new vStack window. The first row already has the glass and air

materials correctly set up. The coating for the first surface is added to the interface by double-clicking in the Coating File. This will cause a file chooser to be displayed. Select the chevron coating file. You can either double-click the file name or click Open to add the coating file to the vStack. There are two ways that the coating can be applied to the surface. The layer next to the medium in the design can go next to the front material of the surface or it can go next to the back material. These two possible orientations are controlled by the value in the Coating Direction column. When the direction is set to Forward, the layer next to the medium in the design is next to the Front Material in the vStack. When the direction is set to Reverse, the layer next to the medium in the design is next to the Back Material in the vStack.

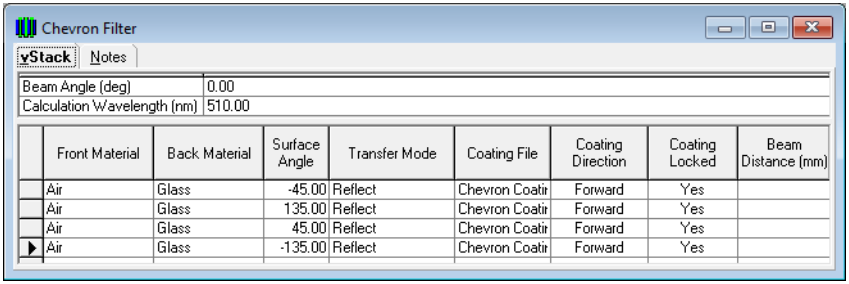
The angle of the first surface now needs to be defined. Referring to the layout diagram above, the surface angle (the angle of the normal to the surface) of the first surface is –45 degrees (or 315 degrees) relative to the reference direction. Enter the value into the Surface Angle column.

When the light beam strikes the surface, there are two resultant beams – the transmitted beam and the reflected beam. The beam that we wish to use is the reflected beam. Click in the Transfer Mode cell until Reflect is visible. This instructs vStack to take the reflected beam from this interface.

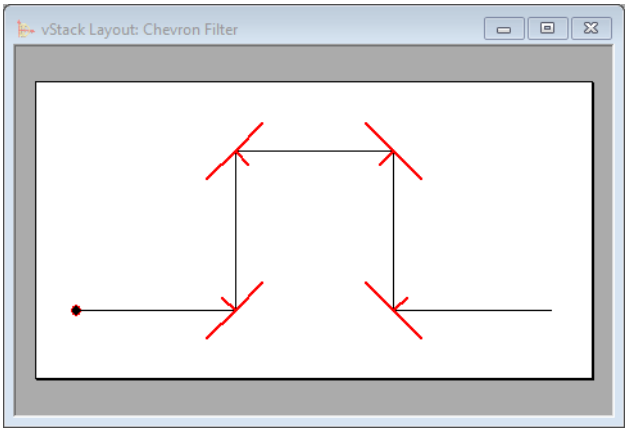
The first interface of the chevron filter should look like the figure below



To complete the chevron filter, we need to add the three remaining interfaces. With the Essential Macleod in insert mode (the panel at the bottom of the Essential Macleod window shows the value Insert), press <Enter> repeatedly until a new line is created in the vStack window. This line can be edited in the same way as the first line. The only difference is the change in the surface angle. For the second interface, the surface angle is 135 degrees as can be seen from the layout diagram above. The third and fourth interfaces are entered in the same manner. The completed chevron filter should look like the figure below



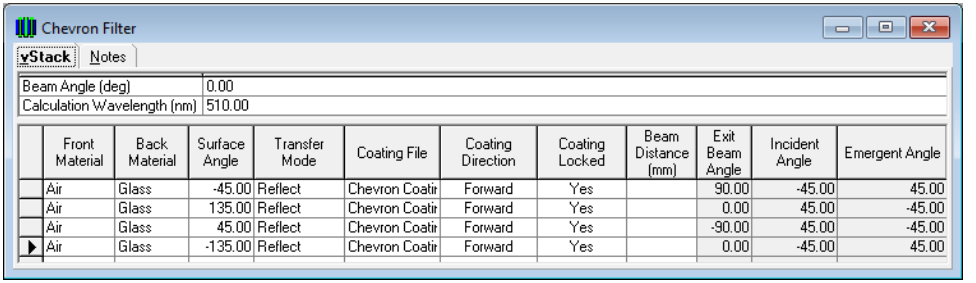
We check that the vStack has been correctly defined by using the Draw Layout command. Click the **Tools** menu and select **Draw Layout**.



The light beam starts at the black circle. A red line represents each interface. A small red line perpendicular to the large red line defines the front surface of the interface. Comparing the layout to the picture at the start of this section, we can see that the filter has been correctly defined in vStack.

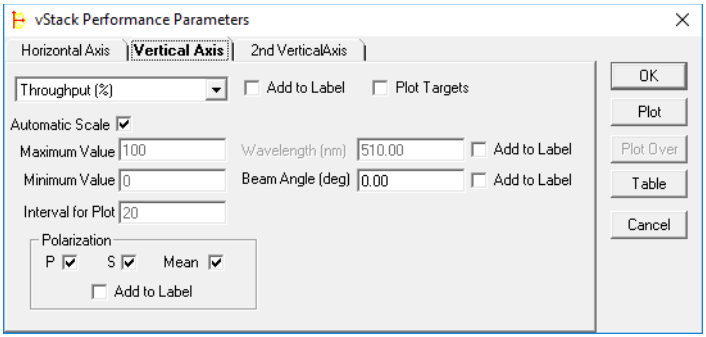
If the **Auto Draw Layout** command in the Tools menu is checked, then the layout will be updated after each change to the vStack.

The incident and emergent angles of the beam on each of the coatings can also be displayed. From the **File** menu, select **Display Setup >**. A sub-menu will appear. Select **Beam Angle Data** and click **Close**. This will cause three columns to be added to the vStack window. These columns show the beam angle of the light exiting the surface, as well as the incident and emergent angles of the beam with respect to the normal to the surface.



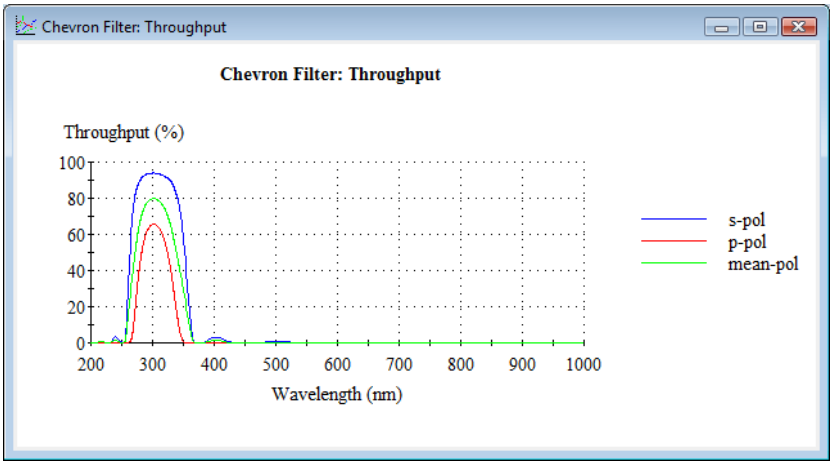
	Front Material	Back Material	Surface Angle	Transfer Mode	Coating File	Coating Direction	Coating Locked	Beam Distance (mm)	Exit Beam Angle	Incident Angle	Emergent Angle
	Air	Glass	-45.00	Reflect	Chevron Coatir	Forward	Yes		90.00	-45.00	45.00
	Air	Glass	135.00	Reflect	Chevron Coatir	Forward	Yes		0.00	45.00	-45.00
	Air	Glass	45.00	Reflect	Chevron Coatir	Forward	Yes		-90.00	45.00	-45.00
▶	Air	Glass	-135.00	Reflect	Chevron Coatir	Forward	Yes		0.00	-45.00	45.00

Now we set the performance parameters by selecting **Performance...** from the **Parameters** menu.



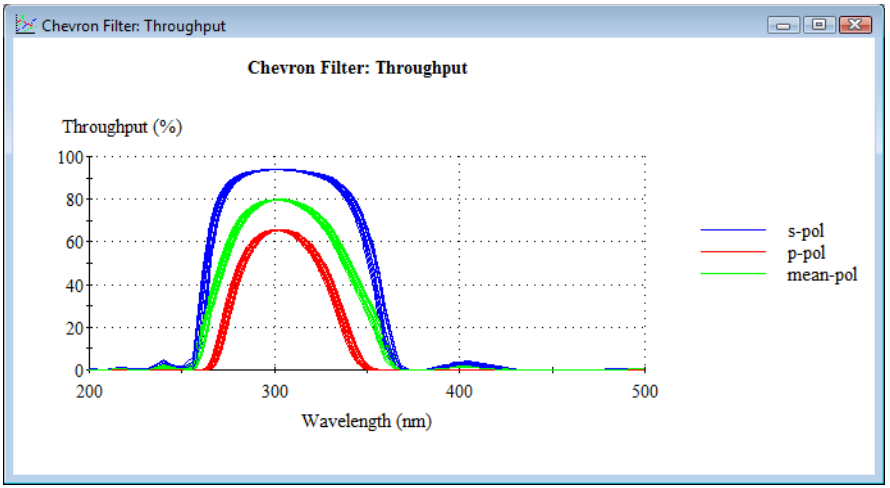
The **vStack Performance Parameters** dialog box is similar to others in the package. Once the parameters are considered satisfactory, the plot and/or table can be calculated. Selecting **Plot** in the **Performance** menu gives the following graph. This is the transmission (throughput) of the chevron filter.

The vStack and its performance can be saved in the normal way.



The impact of errors on the performance of a vStack can be assessed in a similar way to that of a Design. vStack has its own set of errors independent from those attached to a Design. The errors are specified as statistical parameters to be applied to the layers in the Designs used by vStack. Where a Design is used more than once in a vStack, the same perturbed Design will be used at each surface in the vStack, that is, the errors will be 100% correlated for each Design appearing more than once in the vStack. (To consider the zero correlation case, create a copy of the Design for each time it appears in the vStack and change the designs in vStack so that each surface has its own separate copy of the Design.)

The plot below shows the results of 1% standard deviation errors applied to ZrO2 and 2% standard deviation errors applied to SiO2 for the chevron filter.


Chevron Filter: Throughput
Chevron Filter: Throughput
Throughput (%)
100
80
60
40
20
0
200
300
400
500
Wavelength (nm)
s-pol
p-pol
mean-pol

FUNCTION

The Function Enhancement adds the potential to carry out a virtually unlimited range of extra calculations. Coatings may be used under special conditions of illumination. Thermal emittance or absorptance may be needed. Performance may be required of combinations of coated components with differing angles of incidence, where some are transmitting and some reflecting, and where source or receiver may have a particular spectral variation. The core tools can provide the performance data needed for such calculations, but performing them can be tedious and clumsy in contrast with the simplicity of carrying out the basic performance assessments. Function is designed to performs such calculations. It has two separate features. Operations use a simple macro language for rapid, straightforward manipulations that take table files and reference files as input. Scripts use a powerful version of BASIC that can define most of the entities in the Essential Macleod as objects. Operations are quicker and easier to write but are more limited in their capabilities than scripts.

In appearance and operation, Function is similar to the rest of the package You can check whether or not the Function Enhancement is present by starting the Essential Macleod and selecting **About The Essential Macleod…** in the **Help** menu. The information box that appears should list Function against the Options. If, however, you have just received the Function Enhancement as an upgrade to an existing installation then you will need to obtain a new Site Key.

Scripts

A script can be called whenever a document that supports a script is open and active or when the application window is empty. Scripts are called through the Script Manager, opened by clicking **Scripts** in the **Tools** menu. The Script Manager shows the available scripts and a series of options permitting running, editing or creating new scripts, and manipulating the list. Most scripts supplied with the Essential Macleod also have help files in pdf format that describe their function and use. The Help button accesses them, provided a pdf reader is present. Frequently used scripts can be given their own menu entry in the Tools menu. See the Scripts topic in the help for more information. The scripting language is fully described in the Scripting Language User Guide. This is accessible through the item Essential Macleod Help in the Macleod folder in the Start Menu, or through **Scripting Help** in the **Help** menu whenever a script is open for editing. The help for scripts is in the Scripting Language book at the bottom of the contents list. The remainder of this chapter deals with Operations.

Function Menu

The screen layout is exactly similar to that of the Essential Macleod. Apart from **Scripts** in the **Tools** menu, the only immediately visible differences when the Application window is active are in the **File** menu where there is an additional item **Open Function**. The menu item **New...** in the **File** menu has, in fact, also changed with the addition of **Operation** as one of the choices. We deal with the **Options** menu first.

Options Menu (Application)

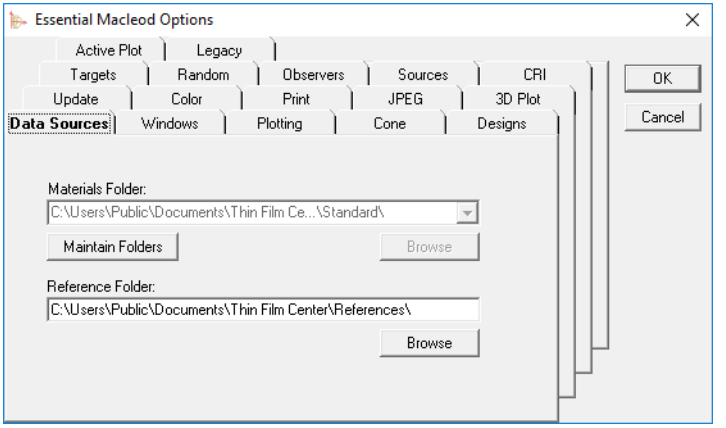
General

The **General** option has already been described in connection with the Core Program but some mention is necessary in connection with Function. Function operates on the basis of instructions that frequently include reference data. A set of instructions is known as an Operation and is stored in an Operation file. Reference data are stored in Reference files. The folder where these Operation and Reference files are stored is known as the Reference Folder. Since the files are identifiable by their extensions, any folder is capable of serving as the reference folder. We suggest however, that a separate standard folder be maintained containing a complete set of reference and operation files. Those necessary for a project may then be copied into the local project database that may also contain materials, substrates, designs and other data files and that may then be declared as the reference folder. This will insulate the standard folder from any local changes. As always, a small amount of effort on the part of the user in maintaining order will pay off handsomely.

Note that the color functions in the Core Program require the existence in the current reference folder of a number of color reference files. These must also be present in the reference folder should it be different from the standard one.

The usual folder will be …\References\ and this will have been automatically created and supplied with some standard files during installation. If Function has just been installed as an upgrade then the new references and operations supplied with it will have been installed in a separate reference folder usually with the name …\References0\. This new folder will contain also the necessary standard color files - although any local changes made by the user will not be included.

The reference folder is specified in the General Options dialog box by entering it in the appropriate field.



Reference files are exactly what their name suggests. They contain data that is necessary for the calculations that will be carried out. Since their data is of a more or less permanent nature, they are called reference files. Typical reference files contain the

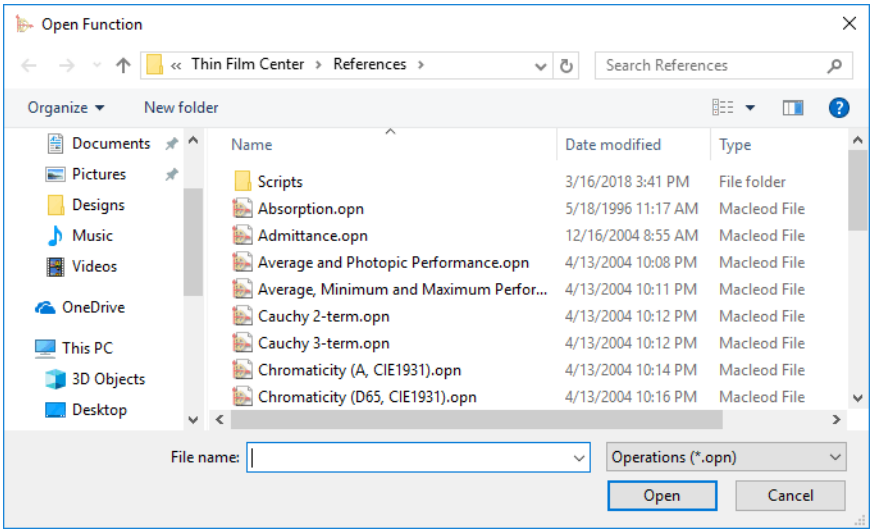
tristimulus functions, the spectral variation of standard illuminants, and so on. They can be examined and edited, but this should not be done casually.

Operation files contain instructions for performing calculations. They consist of a set of functions that are specified in a form that will be described, along with a list of reference files and other constants that will be used, and a list of the data that will be manipulated. To perform an operation, its instruction file must be loaded and then executed. A number of useful operations is provided with the enhancement and some of these will be described in greater detail shortly.

Open Function...

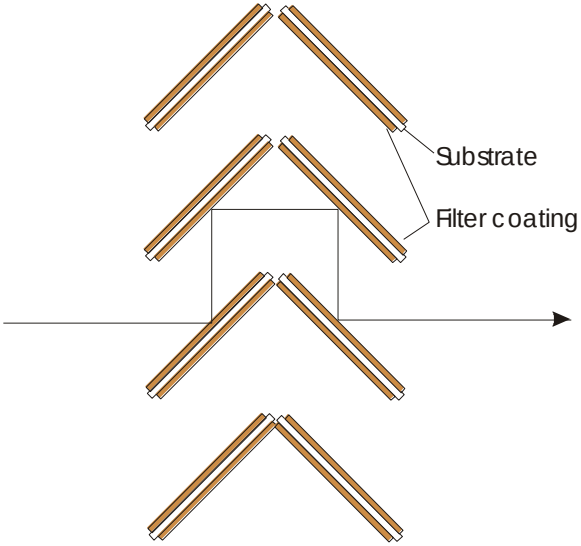
Open Function in the **File** menu permits the selection either of operation files or of reference files according to the **List Files of Type** drop down menu. The extensions that apply are **.opn** and **.ref** respectively.

Note that this is the only way of loading a reference file for examination or plotting or for editing. Reference files are by their very nature to be preserved and so their manipulation is deliberately made less convenient than other files.



An Example: Chevron Filter

When an image is not necessary, a useful type of filter particularly in the ultraviolet part of the spectrum is based on a chevron arrangement. The overall filter works in transmission but its mode of operation consists of four successive reflections at 45°. The filter is shown schematically in the figure below.



The substrates are opaque so that the product of the four reflections gives the performance of the device.

The Core Essential Macleod does not handle this type of calculation. We now show how readily it may be performed by Function.

We will calculate the overall performance of the filter and then make a further calculation of the spectral variation of the output of the filter when illuminated by a source with given spectral characteristics. For simplicity, we will assume a D65 source, which represents daylight in the middle of the day.

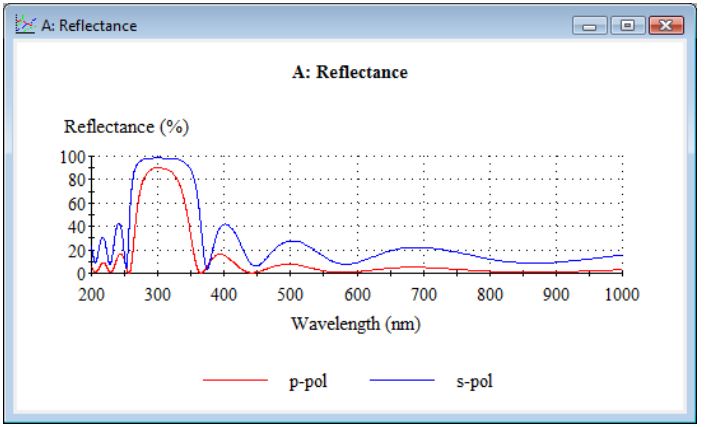
First we design the filter. This is an 11-layer quarterwave stack centered at 300nm corrected by Match Angle for 45°, and constructed from silica and zirconia on a substrate of glass. The glass can be chosen to be sufficiently absorbing across the ultraviolet, visible and near infrared or the individual components can consist of slices of glass with blackened rear surface arranged back-to-back. The successive reflections are at 45° and so polarization must be taken into account in the calculations although we shall assume unpolarized light from the source. The filter and its performance are shown next. The results for s- and p-reflectance are calculated at 45° from 200 to 1000nm at intervals of 10nm and the table is saved under the arbitrary name a.tbl.

A

Design | Context | Notes

Incident Angle (deg)	0.00
Reference Wavelength (nm)	300.00

	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
▶	Medium	Air	1.00000	0.00000		
	1	ZrO2	2.15300	0.00216	0.26607307	37.07
	2	SiO2	1.48780	0.00000	0.28564202	57.60
	3	ZrO2	2.15300	0.00216	0.26607307	37.07
	4	SiO2	1.48780	0.00000	0.28564202	57.60
	5	ZrO2	2.15300	0.00216	0.26607307	37.07
	6	SiO2	1.48780	0.00000	0.28564202	57.60
	7	ZrO2	2.15300	0.00216	0.26607307	37.07
	8	SiO2	1.48780	0.00000	0.28564202	57.60
	9	ZrO2	2.15300	0.00216	0.26607307	37.07
	10	SiO2	1.48780	0.00000	0.28564202	57.60
	11	ZrO2	2.15300	0.00216	0.26607307	37.07
	Substrate	Glass	1.55277	0.00001		
					3.02464852	510.43



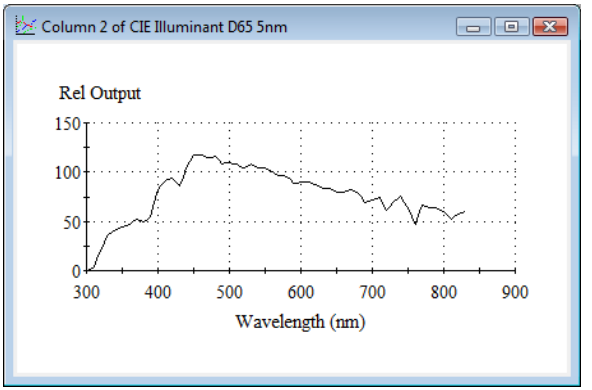
A: Performance

Table | Notes

Design	A
Reference Wavelength (nm)	300.00
Incident Angle (deg)	45.00

Wavelength (nm)	P-Reflectance (%)	P-Transmittance (%)	S-Reflectance (%)	S-Transmittance (%)
200	5.746591	91.307037	22.666273	74.914317
220	8.345041	89.070176	27.266026	70.686218
240	14.430925	83.344360	42.366296	56.098075
260	7.259480	90.214775	69.406966	29.331538
280	81.879559	17.152808	97.422957	2.190545
300	90.016089	9.072497	98.446494	1.144122
320	86.454910	12.285628	97.952153	1.496092
340	61.986915	36.971157	94.774487	4.779473
360	3.553808	95.172642	64.352772	34.479015

The D65 illuminant curve is shown next. This is stored in table ILLUMD65.ref and the values are given every 5nm.



Now to calculate the performance of the filter we must find the product of four such mirrors. We must derive the results for s- and p-polarizations separately and then, for unpolarized light, calculate the mean.

The results are in percentage and if we want to have the final figures also in percent then we multiply the characteristics together but we must also correct by multiplying the product by 0.000001. The calculation can be written as:

$$T_p = 0.000001 \times R_p^4$$

with a similar one for T_s. Then the results should be combined as

$$T = 0.5 \times (T_p + T_s)$$

Then, when we have finally calculated T we can multiply it by the relative output of the source to give the final characteristic of the filter.

In each of these expressions the quantities are functions of wavelength and so we have to repeat each of the operations for each wavelength point.

Next we multiply each of the final transmittance values by the spectral output of the source at the appropriate wavelength. This can be written as

$$R_\lambda = C \times S_\lambda \times T_\lambda$$

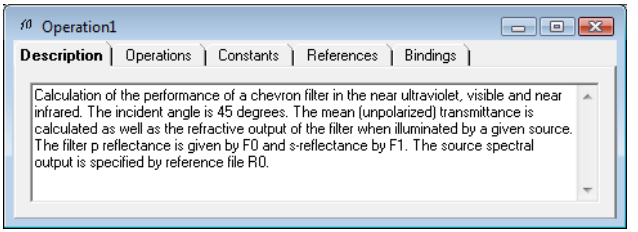
where *C* is a constant that normalizes the result. We shall assume 0.01 for *C*. Since the D65 illuminant curve and the filter are both functions of wavelength, for every calculation corresponding to equation each of the quantities must be referred to the same wavelength.

An Operation consists of one or more Functions. Each Function is an expression like the equations above but the quantities in the Function are assumed to be arrays rather

than simple variables. Further, so that multiplications and other similar operations can be carried out correctly, the arrays are first interpolated, completely automatically, so that the wavelength values are identical.

Setting Up the Operation

We first open the **New** submenu under **File** and choose **Operation**. A new Operation form opens. Since this is a new operation all entry screens are blank. This first one, shown here, is the description screen that will contain a description of the operation. The other screens for entry can be selected by clicking on the appropriate tab. We first type in a description of the operation for future reference. This can be quite long if necessary.

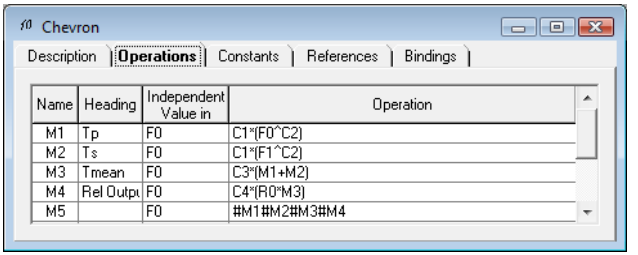


Now select the Operations tab to pass to the entry of the Operation. A blank table appears with three empty columns and rows labeled **M1** to **M9**. These should be completed as follows.

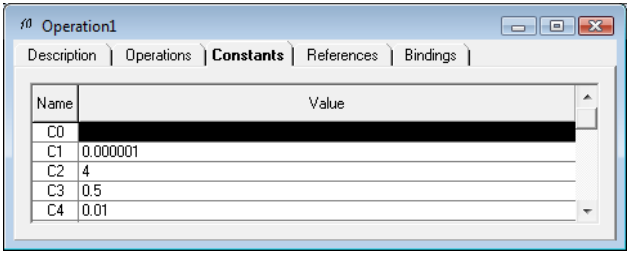
Name	Heading	Independent Variable In	Value
M1	Tp	F0	C1*(F0^C2)
M2	Ts	F0	C1*(F1^C2)
M3	Tmean	F0	C3*(M1+M2)
M4	Rel Output	F0	C4*(R0*M3)
M5		F0	#M1#M2#M3#M4

F0 and **F1** up to **F9** indicate columns in data files. In this particular case, **F0** is the p-reflectance of the basic filter at 45°. **F1** is the s-reflectance of the same coating. **C1**, **C2** up to **C9** indicate constants. Here **C1** is 0.000001, **C2** is 4, **C3** is 0.5 and **C4** is 0.01. **R0** to **R9** indicate reference files and here **R0** is the reference file containing the D65 light source data. The first function is labeled **M1** and calculates the p-transmittance of the overall filter by taking the result **F0**, that is the p-reflectance of the single coating and raising it to the power **C2**, that is 4. The result is then corrected so that it is in percent by multiplying by **C1**, that is 0.000001. Although there is only one result at each wavelength point, nevertheless we have to state the definitive source of the wavelength values to be used for the calculations and that is given as the same file, **F0**. Although **F0** indicates the p-reflectance column, when it is entered into the **Independent Variable In** column it is taken to mean the independent variable in the same file from which **F0** is taken. The independent variable is always in column 1. The next function, labeled **M2** repeats the calculation but for s-polarization. In the third function the symbols **M1** and **M2** indicate the results of the first and second function respectively. Their sum is multiplied by **C3**,

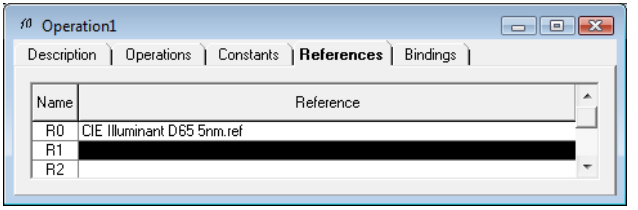
that is 0.5, to find the mean. The mean transmittance, in **M3**, is then multiplied by the source spectral output given by **R0** and normalized by further multiplying by **C4**, or 0.01. Then function **M5** simply means consolidate the results in functions **M1** to **M4** in one single table of results. To do this all results and the table should have the same independent variable and this is satisfied because all have **F0** as the definitive table of wavelengths. The appearance of the table at this stage is shown in the figure.



Now we need to put in the constants. Select the **Constants** tab and complete the table of constants as shown in the next figure. Note that we are omitting **C0** as a designation for a constant. **C0** has a special meaning. It is a constant that is entered at run time and the cell labeled value should actually be completed with the string that will be displayed when entry of the constant is invited.



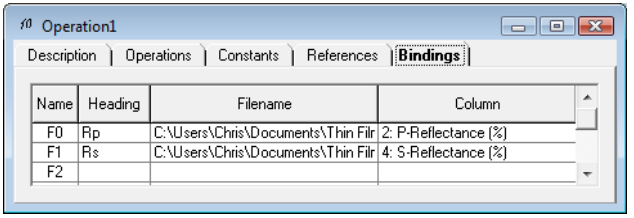
The reference file **R1** is next. Select the **References** table by clicking on the tab. To select the file for **R1** simply double-click in the cell next to **R1** and a selection box will appear. **illumd65.ref** is the correct file here.



Finally select Bindings so that the files **F0** and **F1** can be specified. They are actually columns in the same table. The Default Column can be used as a prompt to remind you of the particular variable that is represented by **F0** and **F1**. If the entry coincides with the heading of one of the table columns, then that column will automatically be identified for

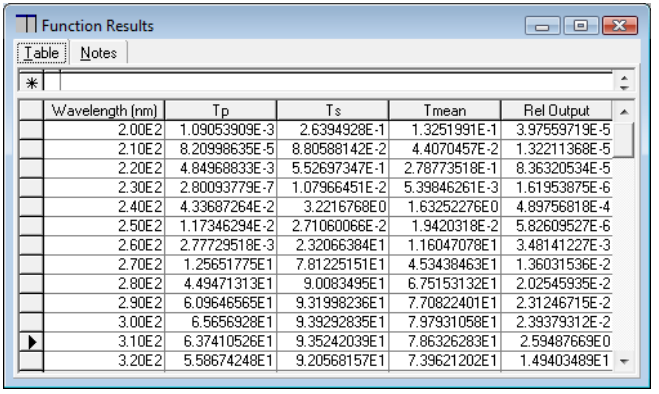
confirmation. Clicking in the Filename cell brings up the usual selection box and clicking in the column cell permits choice of column in the same way as when plotting from a table. The appropriate table in this case is **a.tbl** with columns 2 and 4 as shown.

The assignments that have now been made will be preserved when the Operation is saved but they can also be changed by the user at will.



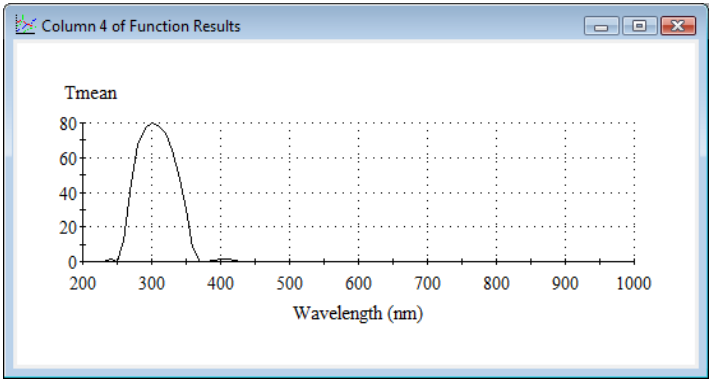
Finally we want to run the Operation. **Execute** is the appropriate menu and the command **Run**.

The table that appears is shown next. We save it under the name **Results.tbl** and we are ready to plot the curves in the usual way.

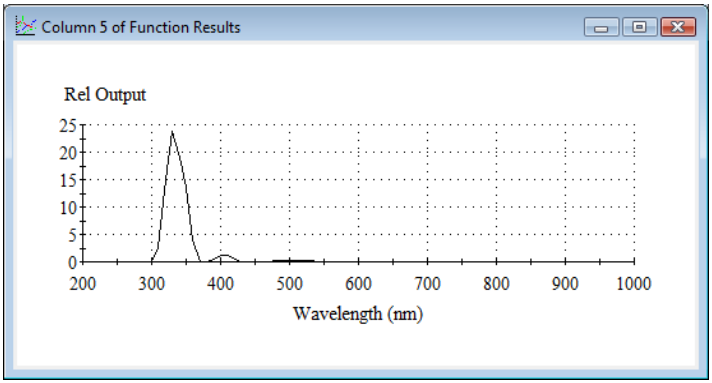


Wavelength (nm)	Tp	Ts	Tmean	Rel Output
2.00E2	1.09053909E-3	2.6394928E-1	1.3251991E-1	3.97559719E-5
2.10E2	8.20998635E-5	8.80588142E-2	4.4070457E-2	1.32211368E-5
2.20E2	4.84968833E-3	5.52697347E-1	2.78773518E-1	8.36320534E-5
2.30E2	2.80093779E-7	1.07966451E-2	5.39846261E-3	1.61953875E-6
2.40E2	4.33687264E-2	3.2216768E0	1.63252276E0	4.89756818E-4
2.50E2	1.17346294E-2	2.71060066E-2	1.9420318E-2	5.82609527E-6
2.60E2	2.77729518E-3	2.32066384E1	1.16047078E1	3.48141227E-3
2.70E2	1.25651775E1	7.81225151E1	4.53438463E1	1.36031536E-2
2.80E2	4.49471313E1	9.0083495E1	6.75153132E1	2.02545935E-2
2.90E2	6.09646565E1	9.31998236E1	7.70822401E1	2.31246715E-2
3.00E2	6.5656928E1	9.39292835E1	7.97931058E1	2.39379312E-2
3.10E2	6.37410526E1	9.35242039E1	7.86326283E1	2.59487669E0
3.20E2	5.58674248E1	9.20568157E1	7.39621202E1	1.49403489E1

The filter response curve is as follows



And the filter relative output



This is badly affected by the abrupt drop in output from the D65 illuminant at 300nm so the response curve is rather narrow compared with the filter response. Also the source peak emphasizes the minor leaks at 400nm, 500nm and 700nm that can just be seen in the plot. A simple redesign of the original filter to reduce the long wavelength ripple would take care of this problem. The advantage of having the Operation established is that a return to the design for some refinement could be followed by the calculation of a fresh table, saved under the same name as before. Then the Operation can be re-executed with no further changes.

Note the usefulness of the ability to define the independent variable scale. For example, to calculate the ratios of the total in-band and out-of-band powers in the filter output we first set up two data files with the appropriate scales. We can do this by taking the results file and deleting all wavelengths outside the band, and then saving it as a new file, **inband.tbl**, say. We have to make a decision on what we mean by in-band and the results will be quite a sensitive function of this choice. Here we take the entire band of the filter between the first minima on either side, the range 250nm to 370nm inclusive.

We then define **F0** as the complete performance of the filter in Column 5 of **results.tbl**, **Rel Output** in the table of results, and we define **F1** as the new file with only the in-band wavelengths. Next we need three functions.

Name	Heading	Independent Variable In	Value
M1	Ttotal	F0	OI:F0
M2	Tinband	F1	OI:F0
M3	Ratio		(M1-M2)/M2

OI: is an operator that means integral. Since it has only one argument it is known as a unary operator. Here in the first function **M1**, it operates on **F0** and integrates it over the range of variable given in the independent variable column of the same file. The second function looks similar and it is except that the range of the independent variable for the integration is now **F1**, the file defining the in-band power. Next we subtract the in-band power from the total and take the ratio with the in-band power to give the final result. (We must do it this way because we cannot integrate over two noncontiguous regions in one operation, which we would need to do to get the out-of-band power directly).

There are different ways of defining stray light. There might be a fixed wavelength interval in a specification and we might be attempting to design a filter system to meet that specification. Then we can set up a file that lists the specified in-band wavelengths instead of taking them from the filter curve we have just derived.

More about Operations

We look further at the Function tab of the Operation.

The first column is the **Name** of the function. There are nine possible functions and their names are always of the form **M*** where ***** indicates an integer from 1 to 9 inclusive. The functions are always evaluated in the order **M1** to **M9**. There can be up to nine functions in an operation.

The second column is the **Heading**. In this set of functions some of the headings are blank. Functions that have blank headings are evaluated only for the purposes of subsequent calculations but the results are not preserved after the operation is completed. The **Heading** is also the label that will be attached to the results that are preserved.

Independent Variable In is the next column. The functions represent manipulations that are to be performed on tables of values rather than individual numbers. An expression like **A*B**, for example, would mean the product of the values entered in two different tables. If we visualize **A** and **B** as two columns of data in cells then the formula means that in each row the value in the cell in column **A** would be multiplied by the value in the cell in column **B**. The cell values will normally be functions of the same independent variable, and the values that are being multiplied together *must* refer to the same independent variable values otherwise nonsense will result. In many thin film (and other) calculations that have to be dealt with by Function, the existing values may not always correspond to identical values of independent variable. Imagine a response curve that is given every 3nm over the range 300 to 700nm and that this response curve must be multiplied by a source output curve that is given every 5nm over the same range. Clearly

one set of values cannot be simply multiplied by the other. First one set must be interpolated to fit exactly with the intervals of the second. Function does this completely automatically. All that is required is that the definitive set of independent variables must be defined and this is the purpose of the **Independent Variable In** column. The entry in the column will be either **F*** or **R*** where ***** indicates a single digit and **F*** indicates the independent variables in a table file and **R*** in a reference file. These files will be further defined in either **References** or **Bindings**.

The final column in this screen is the **Value** of each function. Each entry is in the form of an expression that must be evaluated to yield the **Value**. These expressions involve a number of entities that we will describe shortly but each function may be thought of as a simple statement in a computer program. An example might be

Row M1 OI:(R1*R2*F1)

Translated, this means that the result, designated by **M1**, is equal to the integral over the range of the appropriate independent variable of the product of the data in reference file **R1**, that in reference file **R2** and that in data file **F1**. **F*** always indicates a data file, **R*** a reference file and **C*** a constant.

Note that there is no hierarchy in the operators. The order should be determined by brackets and there is virtually no limit to the nesting that can be accommodated.

Constants are defined by setting the numbers against **C1** to **C9** under Constants. One constant, however, is a little different. **C0** is by convention reserved for a constant that will be set when the operation is executed. The entry that is to be made against it in the table will be in the form of a text string that will be used as a prompt for a value to be inserted. The operation for construction of a black body curve, **makebb.opn**, is an example of the use of a constant entered at execution time - in that case the black body temperature.

The reference files are listed under **References**.

Finally **Bindings** shows the particular data files that are to be used. To identify the data that are to be used in the various calculations, both a file and a column within the file must be identified for each entry in the **Bindings** table. This can be done either before starting execution by filling in the blanks in the table or by answering prompts once execution begins. If the latter course is selected then the prompts will use the text in the **Default Column** together with the appropriate **F*** to help identify the file. Once the file is identified and loaded, if one of the column headings matches the **Default Column** text then that column will be highlighted for selection. Clicking in the **Column** cell is one way of choosing the table column to be used. The other is to execute the operation by choosing **Run...** (or pressing F5) from the **Execute** menu.

Once the calculations begin the progress is shown in a new window. Usually these will appear so quickly that there will be no time to follow them. This is not a problem. The rapid movement of the information shows that calculations are proceeding. Should the operation hang at some point then the halted display will give a good indication of the point where trouble occurred. For trouble-shooting of the results a Single Step command is provided. This will step through the instructions one by one giving also the opportunity to examine intermediate results.

In the calculation the function expressions F1, F2, R1, R2… are replaced by symbols A1, A2, A3… These indicate arrays in which the values have been appropriately

interpolated. The various stages of the calculations are taken in turn with some of the arrays receiving the intermediate results while the others are discarded. Only if the values are constant will the A be replaced by a C. Note that the integer parts of the array and constant names are not necessarily related to those in the original expressions. They are chosen simply in order of creation.

Writing an Operation

Writing an operation is fairly straightforward. Each operation consists of a series of functions, up to nine in number, that manipulate data files, reference files and constants. Each function consists of an expression that represents the particular calculation it has to perform. The function is identified by a name of the form **M***, where * is a digit, and possibly by a heading. A heading indicates that the results are sufficiently important to deserve saving at the end of the operation. The absence of a heading indicates that the results are to be considered intermediate only.

The parameters of the mathematical expression consist of arrays of data, operators, constants and brackets. Arrays of data are represented by the symbols **F1**, **F2** etc, or **R1**, **R2** etc. **F1** represents data in a data file that will be chosen when the operation is performed. **R1** represents data in a reference file that will be identified when the operation is created. The symbols *****, **+**, **-**, **/** and **^** have their usual meaning. They are binary operators; because they indicate an operation involving two arrays of data. A rather special binary operator is the comma. It indicates arc tangent of the quotient of the quantities on either side of it. **F1,F2** for example, means arc tan(**F1**/**F2**). The reason for the use of the comma is to preserve the quadrant of the result, which is assigned on the basis of the signs of **F1** and **F2** separately. Both **F1** and **F2** positive implies first quadrant, both negative means third quadrant, **F1** negative and **F2** positive is fourth quadrant and **F1** positive and **F2** negative is second quadrant. Then there is a series of unary operators; that involve the transformation of a single array of data. These all have the form **O#:** where **#** indicates a letter and they include operators such as **OS:** for sum. Brackets are used to define the hierarchy of calculation. In the absence of brackets this is principally from left to right but on occasion this may not be so. Brackets should, therefore, be freely used. **C1**, **C2** and so on represent constants. **M1, M2** and so on represent the results of the functions. The result of an earlier function can be used in a later one simply by including the appropriate **M1**, **M2** etc.

One version of the **C** symbol and one of the **M** symbol have special meaning. The symbol **C0** is reserved for a constant that will be input when the operation is being performed. The symbol **M0** means the independent variable of the particular function. It is used, for example, to extract the wavelength so that it can be used as a variable in a calculation. The operation that creates the output of a black body source, supplied with the program, shows an example of this. The **M** symbol can also be used to indicate that the independent variable should, after calculations are completed for a particular function, be replaced by the dependent variable of a previous calculation.

The various symbols are listed in the following table. In all cases ***** indicates a numerical digit and **#** a single letter.

Symbol	Meaning
	Arrays of data
M*	The result of a particular function. Used in the independent variable column indicates that the independent variable of **M*** should be used for the calculation but then should be replaced in the table of results by the dependent variable **M***
M0	The independent variable in the given function
R*	A reference file
F*	An array of results in a table file
C*	A constant
	Binary operators
*****	Multiplication
+	Addition
-	Subtraction
/	Division
^	Exponentiation
,	Arc tangent
%	Search for level from beginning
@	Search for level from end
	Unary operators
OD:	Derivative
OI:	Integral
OS:	Sum
OV:	Mean
ON:	The number of values
OL:	Log (natural)
OE:	Exponential
OQ:	Square root of absolute value
OP:	Principal value in the range -180° to +180°
OB:	Principal value in the range 0 to 360°
OG:	Absolute value
OH:	Sine
OU:	Cosine

Symbol	Meaning
O>:	Maximum value
O<:	Minimum value

Notes: The derivative at a point is given by the difference between the values of the independent variables on either side divided by the corresponding difference between the independent variables. At the beginning or end of a table the missing point is replaced by the point in question.

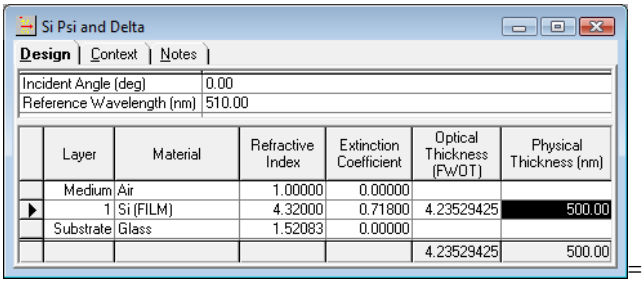
The integrals are evaluated by the trapezoidal rule.

Search for level from beginning and Search for level from end operators
These operators are used to find the value of the independent variable at which the dependent variable has a specified value. Search for level from beginning starts at the beginning of the table and returns the first matching value. Search for level from end starts at the end of the table and returns the first matching value. For example, the operation C1%F1 with Independent Value in F1 returns the Independent Value of the first point in F1 where its value is equal to C1

A particularly useful aspect of the **M** symbol is the way in which it can be used to connect the variation of two dependent variables, each dependent on the same independent variable. An example of this occurs in **delvspsi**, an operation for the rearrangement of the ellipsometric parameters ψ (psi) and Δ (delta). Although these parameters are calculated in the Core Essential Macleod there is no facility for tabulating or plotting Δ against ψ in the Core. Both ψ and Δ are calculated as functions of a third variable, wavelength, layer thickness or angle of incidence. Often the variation of one with respect to the other, especially as the thickness of a layer increases, is what is required. This is achieved by the use of two functions. The first calculates Δ as a function of the original independent variable and also corrects the principal value range to 0 to 360°. This correction could be removed or changed. The second function then sets ψ against the dependent variable of the first function by placing **M1** in the Independent Variable In column.

Name	Heading	Independent Variable In	Value
M1	Della	F0	OB:F0
M2	Psi	M1	F1

A very simple example of the use of this Operation might be ψ and Δ for a silicon film deposited over a glass substrate at a wavelength of 500nm and angle of incidence of 70°. We would like to construct a plot of ψ against Δ. The design is set up as shown and then Reflectance Delta is chosen in the Parameters dialog to be tabulated as a function of the thickness of layer 1.


Si Psi and Delta

Design | Context | Notes

Incident Angle (deg)	0.00
Reference Wavelength (nm)	510.00

	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
	Medium	Air	1.00000	0.00000		
▶	1	Si (FILM)	4.32000	0.71800	4.23529425	500.00
	Substrate	Glass	1.52083	0.00000		
					4.23529425	500.00

=

This is calculated over the range 0 to 250nm of layer 1 to give the table of results, which we save in file **sipd.tbl**.

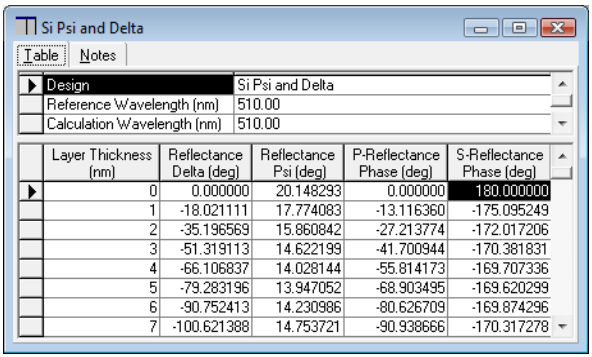

Si Psi and Delta

Table | Notes

▶ Design	Si Psi and Delta
Reference Wavelength (nm)	510.00
Calculation Wavelength (nm)	510.00

	Layer Thickness (nm)	Reflectance Delta (deg)	Reflectance Psi (deg)	P-Reflectance Phase (deg)	S-Reflectance Phase (deg)
▶	0	0.000000	20.148293	0.000000	180.000000
	1	-18.021111	17.774083	-13.116360	-175.095249
	2	-35.196569	15.860842	-27.213774	-172.017206
	3	-51.319113	14.622199	-41.700944	-170.381831
	4	-66.106837	14.028144	-55.814173	-169.707336
	5	-79.283196	13.947052	-68.903495	-169.620299
	6	-90.752413	14.230986	-80.626709	-169.874296
	7	-100.621388	14.753721	-90.938666	-170.317278

F0 is now set to column 2, **Reflectance Delta** and **F1** to column 3, **Reflectance Psi**.

Then we execute the Operation to obtain two tables. The first table we discard. The second table, which has Delta in the first column and Psi in the second, we keep by saving as pd.tbl.

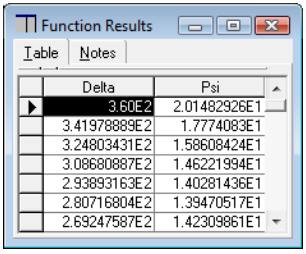
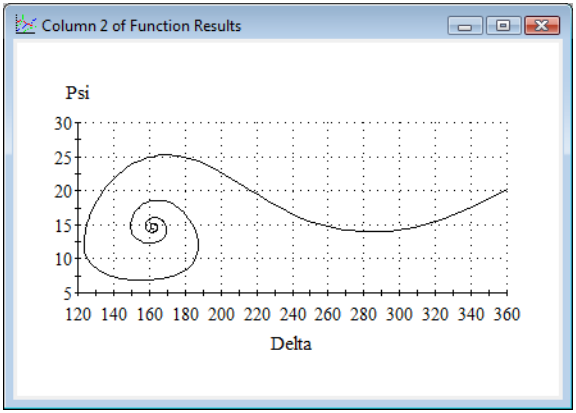

Function Results

Table | Notes

	Delta	Psi
▶	3.60E2	2.01482926E1
	3.41978889E2	1.7774083E1
	3.24803431E2	1.58608424E1
	3.08680887E2	1.46221994E1
	2.93893163E2	1.40281436E1
	2.80716804E2	1.39470517E1
	2.69247587E2	1.42309861E1

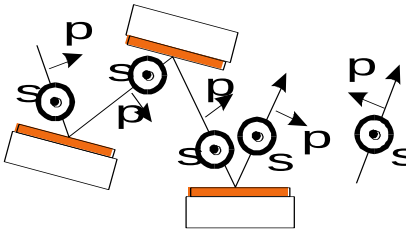
The first value of Delta in the table is actually zero as calculated, but, when we plot this, it places the first point over to the left of the remainder of the curve. So we adjust it by toggling the read only status of the table using the table **Edit** menu and then changing the first entry from 0.0000 to 360. This is the table that we show here.

Finally we plot the result using the **Plot Column** command in the **File** Menu to give the curve shown.



A Further Example

To end this introduction to Function, we consider the generation of a simple operation. Let us calculate the effect of three reflections in series at coated mirrors in an optical instrument. We assume that the light path remains in the horizontal plane, as in many optical instruments and that the three reflections making up the light path follow the shape of the letter W. Since oblique incidence is involved we will have to keep track of the p- and s-performance separately. We will calculate both the reflectance and the phase. Absolute phase is, of course, meaningless in this operation, but we are interested in the relative phase shift between s- and p-polarization. We will use the ellipsometric convention to express the difference in phase between the components.



The arrangement of the beams and the various reference directions associated with the three reflections are shown in the figure. The convention shown on the rays is the normal thin films convention that is followed throughout the package. The ellipsometric convention is shown to the right of the final ray and there is a difference of 180° in the positive direction for p-polarized light.

We are going to include the possibility of different angles of incidence for each reflection and so we assume three table files, each with data applying to one reflection.

As far as the operation is concerned, each separate set of data will be considered as a different data file, even although they may actually be different columns in the same file.

Since we have three p-reflectances, three s-reflectances, three p-phases and three s-phases we have twelve data files in all. One operation can have only ten files, **F0** to **F9**, and so for reflectance and phase we must use two operations. One can be for reflectance and the other for phase.

Again we emphasize that the absolute phase shift for either s- or p-polarization is lost because we cannot include the total paths but the difference between s- and p-polarization will be valid and this is really what we require from the calculations.

We first consider reflectance. For convenience we show the entire operation in tabular form below. This is entered into a new operation form by following these instructions. We first select **Operation** from the **New...** menu item in the **File menu.**

The data files can be designated **F1**, **F2** to **F6** and we will assume that the independent variable, wavelength, is defined by file **F1**. The s-polarized reflectance we can denote by **R(S)** and this will be given by the product of the s-polarization reflectances for each of the three reflections. A similar expression will exist for the p-polarized reflectance, **R(P)**. But the tables will be given in percentages and the final answer should be also given as a percentage. This implies that we must also correct the result by dividing by the square of 100 so that the product of three hundred percent reflections will be simply one hundred percent. Thus

R(S)=C1*(F1*F3*F5)
R(P)=C1*(F2*F4*F6)

where the files containing the s-polarization results are **F1** for the first reflection, **F3** for the second and **F5** for the third, and, correspondingly, for p-polarization, **F2**, **F4** and **F6**. **C1** is a constant with value 0.0001. To enter this function, we select **New...** from the **File** menu and specify **Function** in the resulting dialog box. As the description (the first radio button in the Function window) we simply enter:

Triple reflection - R(S) and R(P)

Next we must enter the functions themselves. These must be of the form:

Name	Heading	Independent Variable In	Value
M1	R(S)	F1	C1*(F1*F3*F5)
M2	R(P)	F1	C1*(F2*F4*F6)

The files for the independent variables must also be entered. The independent variable values can be in any of the existing data files, in a new data file, in any reference file, or the appropriate function may have a single value as result, in which case there will be no independent variable. Here, existing files are **F1** to **F6** and any of these can be entered. A new file would be indicated by any of **F7** to **F9**, a reference file by **R1** to **R9**. The names of the data files will be entered when the operation is performed but any reference file names will form part of the stored operation. For the current operation, **F1** is a good choice for both functions.

Next the constants must be entered. There is only one in this operation, **C1**, which has a value of 0.0001.

There are no reference files in this operation and so we can safely ignore that screen.

Finally select **Bindings** so that the prompts for the various data files can be set up. These prompts are quite arbitrary and are intended to act as a reminder of the particular data that should be input for the correct implementation of the operation. However, data files may have many columns and if the prompt corresponds to the heading above a particular column, then the program will automatically suggest that particular column as the correct one. This can save a great deal of time when the operation is being set up to be performed. Therefore the heading for the column in the **Bindings** table is **Default Column** although any text string can be entered. We choose entries of **R(S)** for **F1**, **F3** and **F5** will have and **R(P)** for **F2**, **F4** and **F6**.

Once all the prompts have been entered, then a name must be chosen for the operation file where the operation will be saved. This can conveniently be **TRIPLER**.

TRIPLER			
Description			
Triple reflection - R(S) and R(P)			
Functions			
Name	**Heading**	**Independent Variable In**	**Value**
M1	R(S)	F1	C1*(F1*F3*F5)
M2	R(P)	F1	C1*(F2*F4*F6)
Constants			
Name	**Value**		
C0			
C1	0.0001		
Bindings			
Name	**Default Column**	**Filename**	**Column**
F0			
F1	R(S)		
F2	R(P)		
F3	R(S)		
F4	R(P)		
F5	R(S)		
F6	R(P)		

Next we consider phase shifts. The next table shows the details of the operation that must be entered.

For the net phase shifts, ϕ_p and ϕ_s, we simply add the separate phase shifts. It is convenient to have them correspond to a principal range and the operator **OP:** or **OB:** will perform this. However, absolute phase shift calculated in this way is essentially meaningless in the context of three reflections of this kind, particularly because there is an uncontrolled path between each mirror and this is not and cannot be taken into account. This uncontrolled path will, nevertheless, be exactly the same for p as for s-

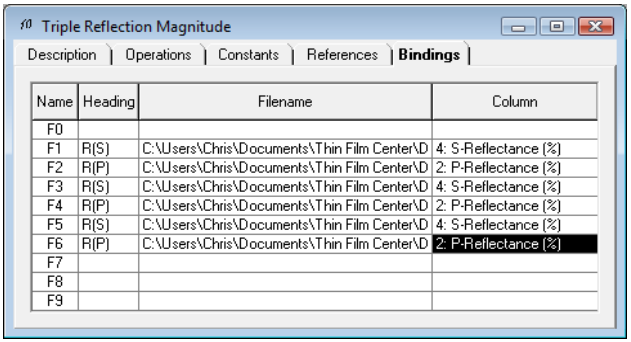
polarization and so the figures we have for absolute phase shifts are completely valid for the calculation of p-shift relative to s-shift. So we calculate the absolute shifts due to the three reflections, but then use the results in the assessment of **DELTA**, the ellipsometric parameter given by the difference ϕ_p-ϕ_s. The operation for phase calculation is shown in the table below and this must be entered in the same way as the reflectance operation and stored in the file **TRIPLEPH**.

TRIPLEPH			
Description			
Triple reflection - PH(S), PH(P) and DELTA			
Functions			
Name	**Heading**	**Independent Variable In**	**Value**
M1		**F1**	**OP:(F1+F3+F5)**
M2		**F1**	**OP:(F2+F4+F6+C1)**
M3	**DELTA**	**F1**	**OP:(M2-M1)**
Constants			
Name	**Value**		
C0			
C1	**180**		
Bindings			
Name	**Default Column**	**Filename**	**Column**
F0			
F1	**PH(S)**		
F2	**PH(P)**		
F3	**PH(S)**		
F4	**PH(P)**		
F5	**PH(S)**		
F6	**PH(P)**		

We are now ready to calculate some actual performance figures. We can choose as reflector, aluminum protected by a halfwave of silicon dioxide at 510nm.

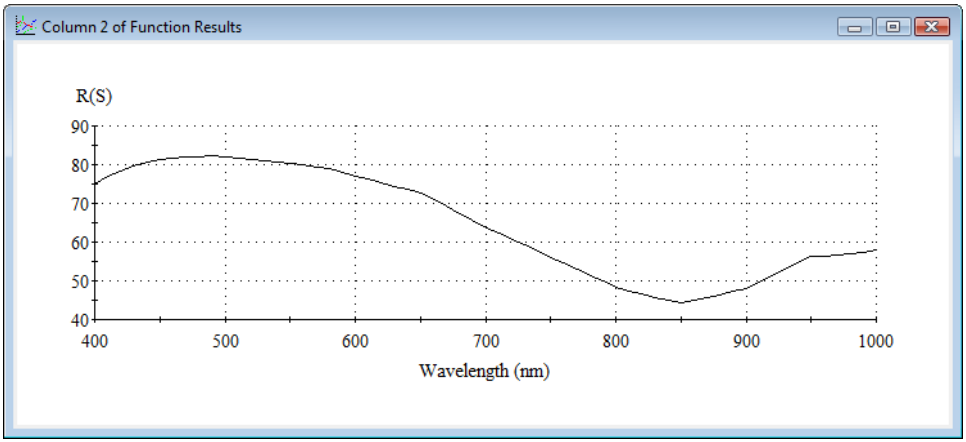
Let the wavelength range be 400nm to 1000nm calculated every 10nm, and let the angle of incidence of the first reflection be 45°, of the second, 30° and of the third, 25°. We set up the calculation parameters for reflectance phase, over the given wavelength range, for 45° angle of incidence and then we calculate the table of results and save it in a table file called **PROTAL45**. In the table of reflectance phase the values of reflectance will also be given. If, however, reflectance is selected in the Parameters dialog box then reflectance and transmittance will be in the table, and this is not what we want. Then we change the angle of incidence to 30°, and calculate the new table, saving the table file as **PROTAL30**. Finally we use angle of incidence 25° and generate the table **PROTAL25**.

Now we make the Operation **TRIPLER** active. We choose the table files as shown in the following screen and we can set them up during execution or before. Note that clicking in the appropriate table cell brings up a dialog box for choosing the appropriate entity.

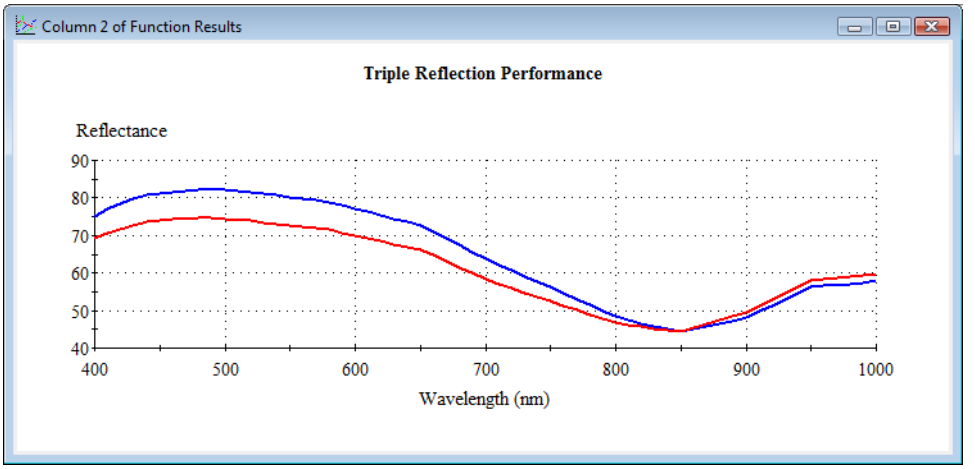


Name	Heading	Filename	Column
F0			
F1	R(S)	C:\Users\Chris\Documents\Thin Film Center\D	4: S-Reflectance (%)
F2	R(P)	C:\Users\Chris\Documents\Thin Film Center\D	2: P-Reflectance (%)
F3	R(S)	C:\Users\Chris\Documents\Thin Film Center\D	4: S-Reflectance (%)
F4	R(P)	C:\Users\Chris\Documents\Thin Film Center\D	2: P-Reflectance (%)
F5	R(S)	C:\Users\Chris\Documents\Thin Film Center\D	4: S-Reflectance (%)
F6	R(P)	C:\Users\Chris\Documents\Thin Film Center\D	2: P-Reflectance (%)
F7			
F8			
F9			

By selecting **Run** from the **Execute** menu we launch the calculations. The results of the calculations are saved as **prals.tbl**, for s-polarization and **pralp.tbl** for p. The plots can then be produced using **Plot Column...** from the **File** menu



To plot one curve over the other on the same graph, save the curve to be added, make the first plot window active by clicking in it and then select the menu item **Add Line...**to add the newly saved plot to the first one.



The reflectance figures are quite low and also quite typical of actual instrumental performance with three reflections.

These two operations can be used over and over again with different reflectors, with different angle of incidence and so on. If they have been saved complete with the bindings then the procedure of generating data and calculating can be speeded up.

RUNSHEET

A Runsheet is a plan for the control of the deposition of a given coating. It lists the expected progress of the signals that are to be used for tracking the progress of the deposition. These signals are normally the output of a monitor that is either a quartz crystal or an optical system or perhaps both.

A Runsheet refers to the production of a particular coating on a given machine. The coating is defined by reference to a normal design file. The significant details of the machine to be used for the production are specified in a document, known as a Machine Configuration.

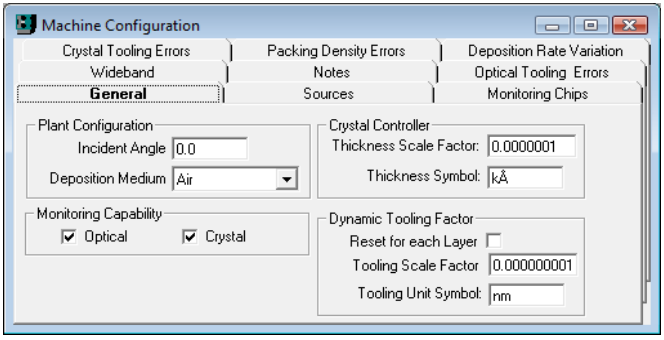
You can check whether the Runsheet Enhancement is present by starting the Essential Macleod and selecting **About The Essential Macleod…** in the **Help** menu. The information box that appears should include Runsheet in the Options list.

Machine Configuration

The submenu activated by **New** in the **File** menu contains an item, **Machine Configuration**. Selection opens a blank Machine Configuration document. It should be completed with the necessary details of the sources and monitoring system of the plant. The example we will show has both optical and crystal monitoring. Either or both of these options may be chosen when the configuration form will show only the appropriate sections. There are four tabs, **General**, **Sources**, **Monitoring Chips** and **Wideband**. **Monitoring Chips** is not accessible when only crystal monitoring is checked. If the Simulator enhancement is installed, then more tabs will be visible. The Simulator section contains details on these tabs.

General Tab

Plant Configuration



Incident angle applies solely to the optical monitor. Polarization of the light for oblique incidence is important and is specified in the Runsheet.

Deposition medium will normally be air (which counts also as vacuum) but the possibility exists to choose any material from the current database.

Monitoring Capability

This must be Optical, Crystal or both. It is not possible to choose neither.

Crystal Controller

The film thickness units used by the crystal controller will often be different from those in the package. Frequently they are in kÅ. They must be specified through the **Thickness Scale Factor** and the **Thickness Symbol** boxes in exactly the same way as in **General Units**. The scale factor is one Machine Unit expressed in terms of the fundamental unit, the metre. For kÅ the **Thickness Scale Factor** will be 1E-07. The mass calibration of the crystal will normally be handled by the crystal equipment. However, if the crystal monitor lacks these facilities, the **Thickness Scale Factor** together with the individual crystal tooling factors can accommodate the entire calibration. Variations in density can also be included in the tooling factors. If optical thickness is specified in the design then, of course, the packing density will be included in the conversion from optical to physical thickness for the Runsheet calculations. However, this will not necessarily represent the entire correction for quartz crystal signal because the crystal thickness conversion ratio will remain constant in the Runsheet but will be altered in reality because of the different density of the deposit.

Dynamic Tooling Factor

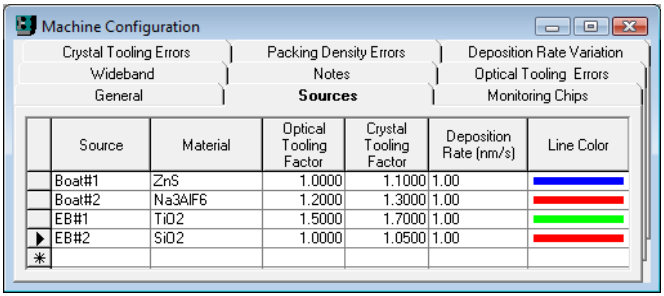
The amount of material deposited on the particular sensor, monitoring chip or crystal, may not be identical to the corresponding amount deposited on the batch of coatings in production. Much of this difference is due to the geometry of the machine and it may be intentional. A greater thickness on the sensor can actually improve the sensitivity and accuracy of monitoring. The tooling factor is defined as the ratio of the rate of deposition on the monitor chip to that on the batch substrates. A **Dynamic Tooling Factor**, described in greater detail shortly, is a function of the total amount of material deposited. Dynamic Tooling Factors can help to compensate for such effects as source depletion during a production run.

Reset for Each Layer is important only when dynamic tooling factors are used. It has no effect if tooling factors are constant. The calculation involves integration of a tabulated function. This calculation can be reset for each layer or can apply without resetting to all layers in sequence deposited from that particular source.

Tooling Scale Factor is another scale factor. This time it applies to the thickness values that are held in the Dynamic Tooling Factor files. It is not used if dynamic tooling factors are not used.

Tooling Unit Symbol is the symbol that represents the thickness units used in the Dynamic Tooling Factor files.

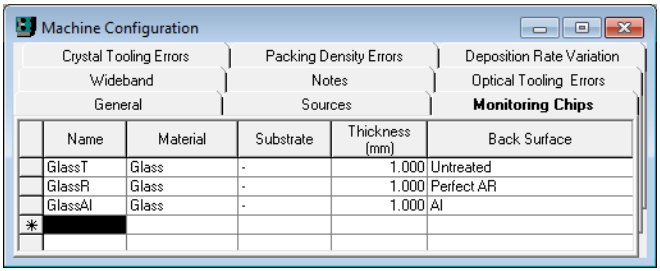
Sources Tab



Sources: The sources are designated by names or numbers. Material can, as usual, be entered manually selected from the drop-down list. **Optical Tooling Factor** expresses the difference between the thickness deposited on the monitoring substrate or chip and the actual substrates carried in the coating jig. A tooling factor greater than unity indicates that the deposit on the monitoring chip is greater than the amount deposited on the substrates. It is the factor by which the thickness of the layer must be multiplied to give the monitor thickness. The **Crystal Tooling Factor** is similarly interpreted. Sources may have varying distributions during the run. This can be accommodated by constructing a dynamic tooling factor. Dynamic tooling factors are described in detail later and involve a table file that is entered in the Tooling Factor cell. The **Deposition Rate** column is used by Simulator and is not used by Runsheet. **Line Color** is used to specify the color on the runsheet plots. To choose the color to be used for each source, double-click in the Line Color cell. A color picker will appear. Select the desired color and click OK.

Monitoring Chips Tab

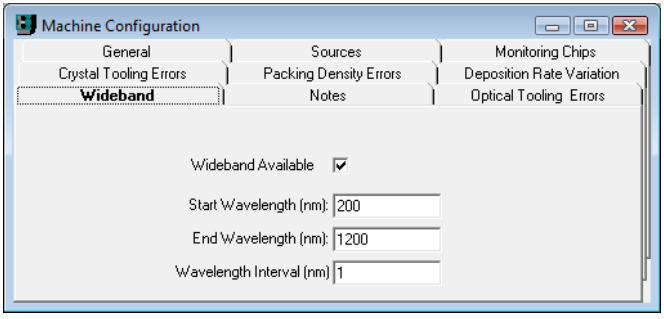
There may be many different monitoring chips. Here we see just three. They may be designated in any way, but a name that includes an indication of the type of chip is most useful. Note the glass chip, **GlassAl**, with opaquely coated rear surface. The rear surface of the chip can have a Perfect AR, to remove any reflection, can be uncoated or otherwise treated, or can have a massive thickness of any of the existing materials added to the rear surface. Usually the coating on such a chip will be metallic and the chip will be used in the deposition of an absorbing film. The example shown has an aluminized rear surface. Each chip may have internal transmittance that is different from unity. Internal transmittance is stored in material files. For older materials databases, the internal transmittance data was stored in a separate Substrate file. In this case, it will be possible to select a Substrate file in the Substrate column. Chip thickness is given in the same units as are used in specifying substrates (millimetres in the standard version) although chip thickness is unimportant when the Material is lossless.



There can be as many machine configurations as the user wishes but it is not possible to have more than one configuration specified in a single Runsheet.

Wideband Tab

The **Wideband** tab specifies the wavelength range and interval to be used for wideband optical monitor calculations.



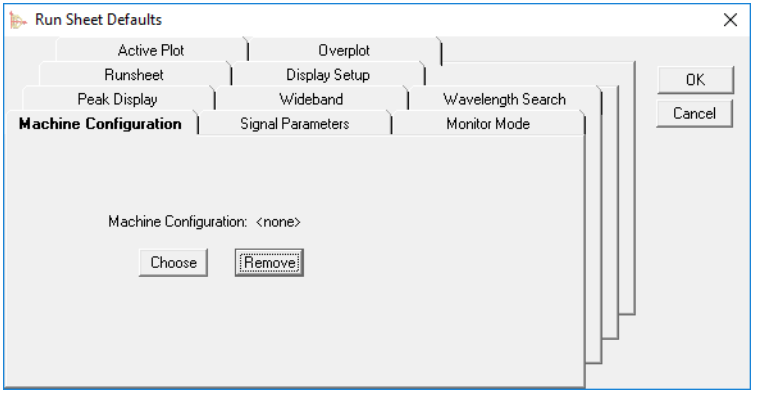
For wideband calculations, wavelengths from **Start Wavelength** to **End Wavelength** incrementing by **Wavelength Interval** will be used.

Run Sheet

Global Defaults

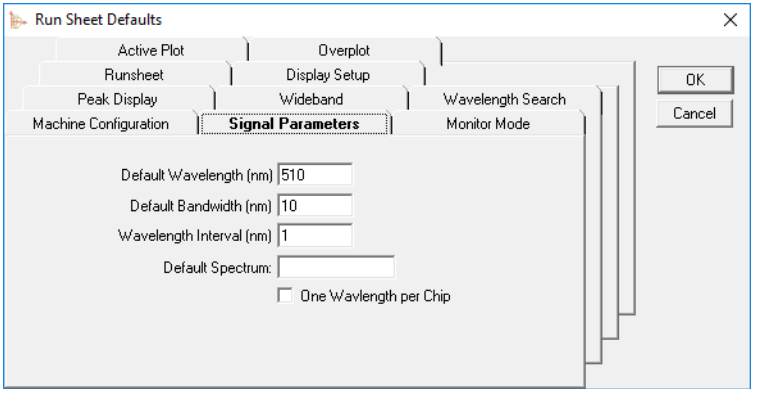
The **Run Sheet…** item in the **Options** menu activates a **Run Sheet Defaults** window with three tabs. [In a Runsheet that has been configured by Monitorlink for a particular controller there may be extra tabs]. Global defaults are to be entered here.

Machine Configuration



The **Machine Configuration** tab permits choice of a default machine configuration. The example shown has no default. If a machine configuration has been chosen and now no default is required then the **Remove** button will return the selection to **<none>**.

Signal Parameters

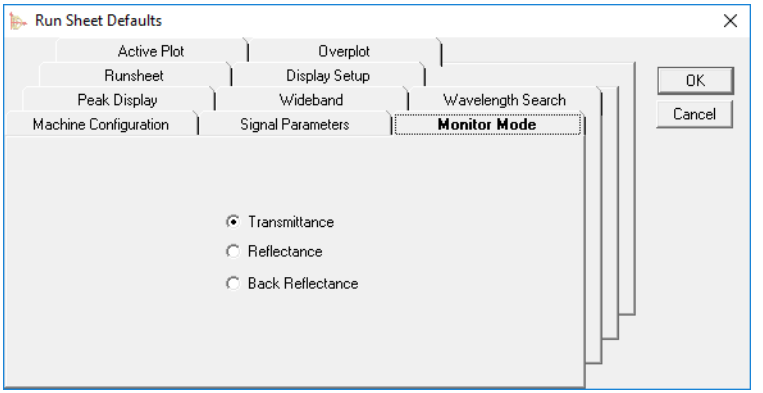


The **Signal Parameters** tab for the regular Runsheet asks for **Default Wavelength**, **Bandwidth**, and **Wavelength Interval**. The bandwidth is the spectral width of the detecting system, filter or other type of monochromator, that will be used. The wavelength interval is, strictly, not a parameter of the particular machine or monitoring system but of the calculation to be performed. It is the interval between those points within the bandwidth of the monitor that will be calculated. The example shown lists 1nm for a bandwidth of 10nm. This means that eleven equally-spaced points will be used in the calculation of the effect of the 10nm bandwidth. This is more than adequate for most purposes. The **Wavelength Interval** should usually be set somewhat less than the **Default Bandwidth**. Note that the minimum number of points that will be calculated, even if the interval is set to be large, will be three, one at either end of the band and one in the

middle. **Default Spectrum** allows you to specify a spectral profile instead of a wavelength and bandwidth

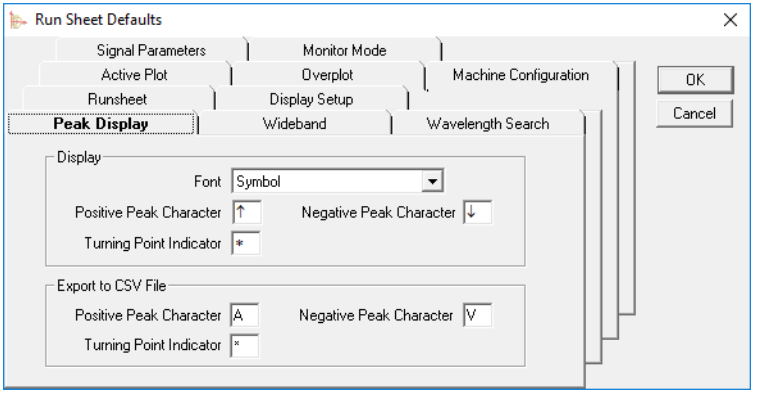
One Wavelength per Chip sets the default behavior of the Runsheet to force the monitoring signal conditions to be identical for all layers deposited on the same witness chip.

Monitor Mode



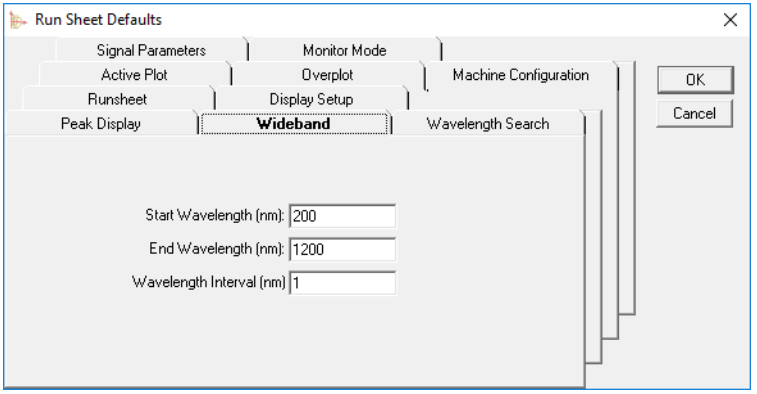
Monitor Mode is transmittance, reflectance or back reflectance.

Peak Display



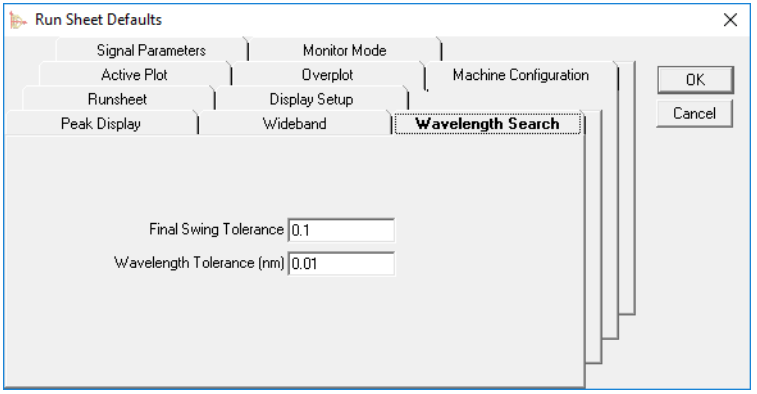
You can specify the characters to use for indicating the signal peaks in the Peak Display page. There are two sets of characters to specify. The first set controls the characters used in the Runsheet window and in printed Runsheets. You can choose a font and then choose characters from that font. This allows, for example, the use of arrows to show positive and negative peaks. The second set controls the characters to be used when exporting the Runsheet data to comma separated values file. Here you can only select standard characters.

Wideband



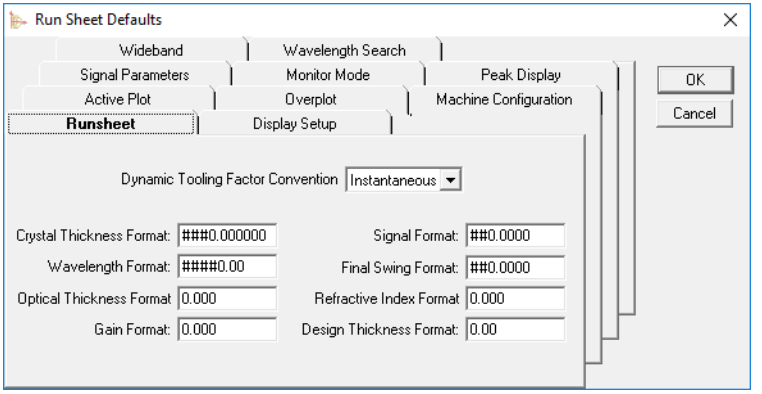
The **Wideband** tab specifies the default wavelength range for new Machine Configuration files for wideband calculations.

Wavelength Search



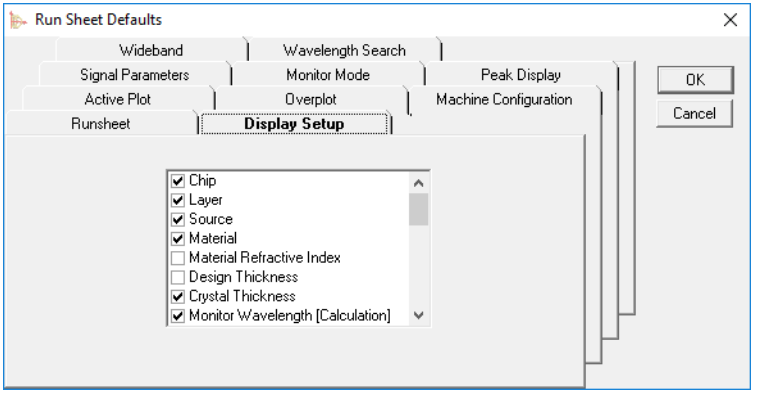
The **Wavelength Search** tab specifies the tolerances to be used during wavelength search. The **Final Swing Tolerance** specifies the accuracy of the match of the requested final swing value to the actual final swing value. The wavelength search function will stop when the calculated final swing is within the **Final Swing Tolerance** value of the requested final swing. The wavelength search function will also stop when the monitor wavelength is within **Wavelength Tolerance** of the wavelength of the requested final swing.

Runsheet



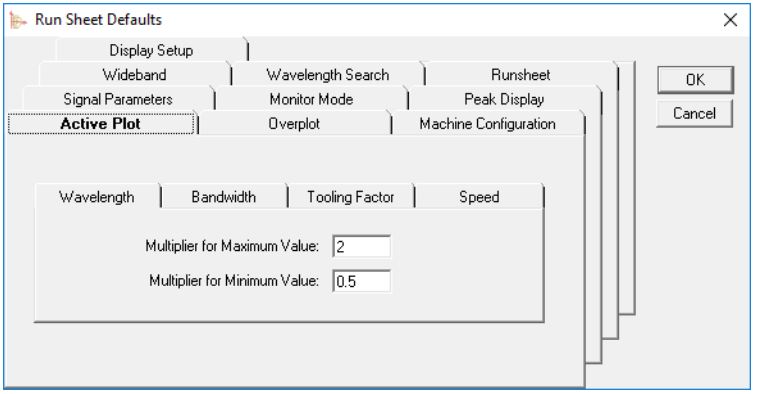
The Runsheet tabs provides controls for the formatting the data that appears on the Runsheet and how the dynamic tooling factor tables are interpreted. The format specifiers follow the same rules as those used in General Units and described in the Units section (see page 32). The Dynamic Tooling Factor Convention controls how the dynamic tooling factor tables are interpreted. For more information on dynamic tooling factor see page 360.

Display Setup



The standard Runsheet has many columns, many of which are probably not required for the majority of Runsheets. This tab controls which columns are initially displayed when a new Runsheet is created. Once the Runsheet is displayed, the columns displayed in that Runsheet can be switched on and off through the **Display Setup** command in the **File** menu.

Active Plot



The Active Plot tab controls the default ranges for Runsheet variables in Active Plot. All the ranges are controlled by multipliers of the initial values. For example, if a Monitor Wavelength variable for a layer was added to a Runsheet Active Plot where the Monitor Wavelength was 510 and the Multiplier for Maximum Value was 1.1, the upper limit of the range would be 561.

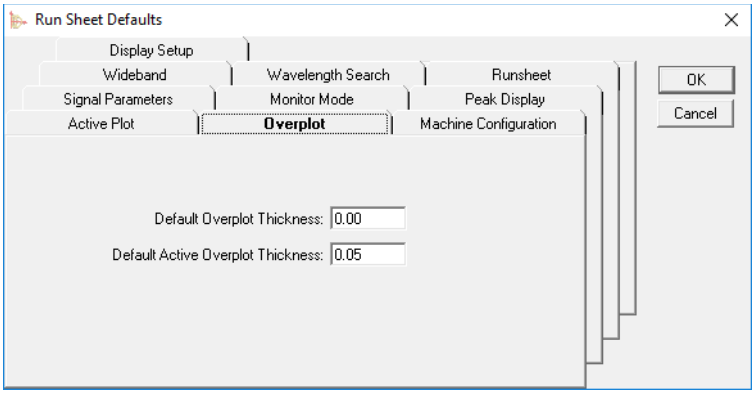
The speed and change increments can also be controlled. When the >, <, >>, << buttons are held down, the Minimum Delay specifies the minimum time period in ms before the variable is incremented and the plot then updated. If the plot update takes longer than the Minimum Delay, then the next plot update will start immediately after the completion of the current plot update.

Each time the > and < buttons increment the value, the value is changed by Increment Proportion of the difference between the maximum and minimum values shown on the Active Plot. The default value is 0.01. That is, the value will change by 1% of the range between the minimum and maximum values.

Each time the >> and << buttons increment the value, the value is changed by Fast Increment Proportion of the difference between the maximum and minimum values shown on the Active Plot. The default value is 0.1. That is, the value will change by 10% of the range between the minimum and maximum values.

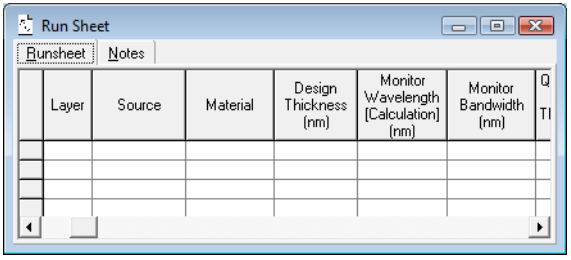
Overplot

The Overplot tab controls the default overplot for each layer in optical thickness units at the monitoring wavelength. **Default Overplot Thickness** controls the overplot for regular plots and **Default Active Overplot Thickness** controls the overplot for Active plots.



Creating a Run Sheet

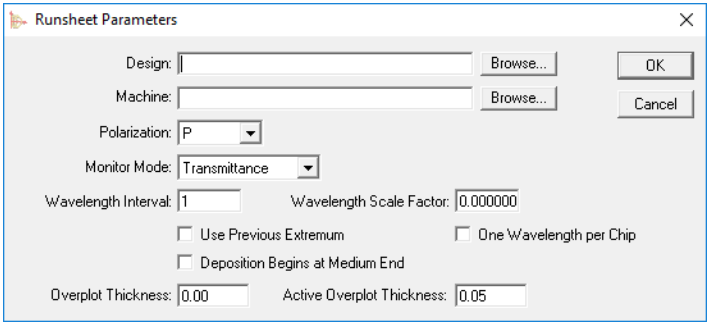
To create a Runsheet, select the **Run Sheet** option in the **New** submenu. A blank Runsheet appears with any global defaults assigned to it. As it is created, the Runsheet is quite broad and will probably need the horizontal scroll bar that is provided.



The commands that we need to proceed are in the Edit and Runsheet menus for the Runsheet. These commands are described below.

Edit Menu (Runsheet)

Parameters...



To specify the design for the Runsheet, click the **Browse…** button or double-click in the **Design** box. A file chooser will be displayed. Select the design file to be used and then click OK. The filename will be displayed in the Design box.

To choose a machine configuration, click the **Browse…** button or double-click in the **Machine** box. A file chooser will be displayed. Select the machine configuration to be used and then click OK. The file name of the machine configuration will be displayed in the Machine box.

For oblique incidence monitoring, a polarization can be specified. Select the down arrow in the **Polarization** box. A list of the polarization options will appear. Choose the desired polarization by clicking on it.

The Runsheet can calculate monitoring signals for transmittance monitoring, reflectance monitoring, or back reflectance monitoring. **Monitor Mode** selects transmittance, reflectance or back reflectance monitoring.

Wavelength Interval is the wavelength step used in the calculation of monitor response over the bandwidth listed against each layer in the Runsheet. This command applies a local default the interval to all layers in the Runsheet. No changes are made to the global defaults.

The **Wavelength Scale Factor** specifies the units used for wavelength in any tables used for defining monitoring spectrum. The scale factor is applied in the same way as for general units. For example, if the scale factor is 1e-9, then the wavelength units of all monitoring spectrum tables will be nanometres. If the scale factor is 1e-06, then the wavelength units of all monitoring spectrum tables will be microns.

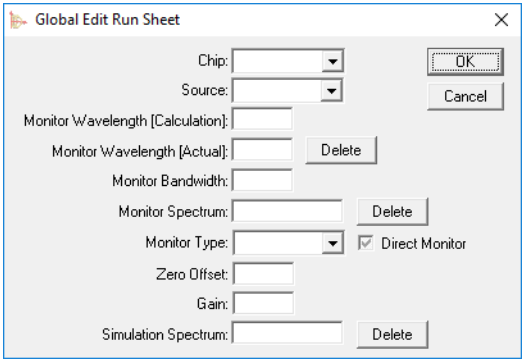
When **Use Previous Extremum** is checked, the Runsheet will use the extrema from previous layers when calculating the Final Swing. Previous extrema are only used when the layers are on the same chip and the monitoring wavelengths and bandwidths (or spectra) are identical.

When **One Wavelength per Chip** is checked, the Runsheet will force all layers deposited on the same witness chip to have the same signal conditions, i.e. the monitoring wavelength and bandwidth will be the same.

Overplot Thickness is the thickness beyond the cut-point for which the signal is plotted on regular plots. **Overplot Active Thickness** is the thickness beyond the cut-point for which the signal is plotted on Active plots. Overplotting helps to determine if the cut-point is near to an extremum or near to some other feature that might cause problems during production.

When **Deposition Begins at Medium End** is checked, the design will be loaded into the Runsheet with the layer next to the incident medium being the first layer to be deposited. Otherwise the design is loaded so that the layer next to the substrate is the first layer to be deposited

Global Edit



Global Edit provides a convenient means for modifying several layers of a Runsheet at once. If no layers are selected, the global edit applies to all layers in the Runsheet. If one or more layers are selected, then the global edit applies only to the selected layers.

Each box on the Global Edit form corresponds to the column of the same name in the Runsheet. Leaving the box blank will leave the contents of the column undisturbed. When a value is entered into the box, the values in the corresponding column will be replaced with the value in the box. **Monitor Spectrum** has a special case. If you wish to delete the current **Monitor Spectrum** entry, click the **Delete** button next to the **Monitor Spectrum** box.

Clicking **OK** causes the global edit to be applied to the Runsheet. Clicking **Cancel** aborts the global edit operation.

Runsheet Menu (Runsheet)

Calculate

This option causes the optical information in the Runsheet to be calculated. The values are displayed in the right-hand part of the table.

Plot One Chip

This option causes the signal variation of the layers deposited on a single chip to be plotted. The chip that is plotted is determined by the location of the currently selected cell. The first chip on or above the row containing the selected cell will be plotted. If there is not a selected cell, then the first chip in the Runsheet is plotted.

Plot All Chips

This option plots the optical signals for all chips on the same plot.

Plot Selected Layers

This option plots the optical signals for selected layers only. Layers may be selected by clicking in the small leftmost cell of a row. The layer is selected when the row has a

black background. Holding the <shift> key down whilst selecting another layer causes all layers between the first selected layer and the new selection to also be selected.

Wideband Plot One Chip

This option plots the expected spectra at the end of deposition of each layer that is deposited on the same chip. The chip that is plotted is determined by the location of the currently selected cell. The first chip on or above the row containing the selected cell will be plotted. If there is not a selected cell, then the first chip in the Runsheet is plotted. The wavelength range to be used in the plot is determined by the Wideband parameters in the Machine Configuration.

Wideband Plot All Chips

This option plots the expected spectra at the end of deposition of each of the layers in the Runsheet. The results for each chip in the Runsheet are shown in separate plots. The wavelength range to be used in the plot is determined by the Wideband parameters in the Machine Configuration.

Wideband Plot Selected Layers

This option plots the expected spectra at the end of deposition of each selected layer in the Runsheet. The wavelength range to be used in the plot is determined by the Wideband parameters in the Machine Configuration.

Wideband Slope Plot One Chip

This option plots the first derivative of the expected spectra with respect to thickness at the end of deposition of each layer that is deposited on the same chip. The chip that is plotted is determined by the location of the currently selected cell. The first chip on or above the row containing the selected cell will be plotted. If there is not a selected cell, then the first chip in the Runsheet is plotted. The wavelength range to be used in the plot is determined by the Wideband parameters in the Machine Configuration.

Wideband Slope Plot All Chips

This option plots the first derivative of the expected spectra with respect to thickness at the end of deposition of each of the layers in the Runsheet. The results for each chip in the Runsheet are shown in separate plots. The wavelength range to be used in the plot is determined by the Wideband parameters in the Machine Configuration.

Wideband Slope Plot Selected Layers

This option plots the first derivative of the expected spectra with respect to thickness at the end of deposition of each selected layer in the Runsheet. The wavelength range to be used in the plot is determined by the Wideband parameters in the Machine Configuration.

Active Plot One Chip

This option begins Active Plot for the signal variation of the layers deposited on a single chip. The chip that is used is determined by the location of the currently selected cell. The first chip on or above the row containing the selected cell will be used. If there is not a selected cell, then the first chip in the Runsheet is used.

Active Plot All Chips

This option begins Active Plot for the optical signals on all chips.

Active Plot Selected Layers

This option begins Active Plot for the selected layers only. Layers may be selected by clicking in the small leftmost cell of a row. The layer is selected when the row has a black background. Holding the <shift> key down whilst selecting another layer causes all layers between the first selected layer and the new selection to also be selected.

Export Signal One Chip

This option creates a csv file containing the signal variation of the layers deposited on a single chip. The chip that is used is determined by the location of the currently selected cell. The first chip on or above the row containing the selected cell will be used. If there is not a selected cell, then the first chip in the Runsheet is used.

Export Signal All Chips

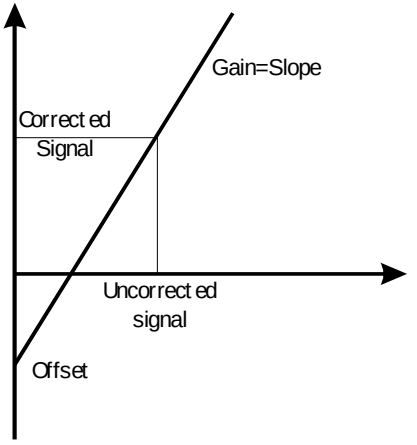
This option creates a csv file containing the signal variation for all chips.

Export Signal Selected Layers

This option creates a csv file containing the signal variation for the selected layers only. Layers may be selected by clicking in the small leftmost cell of a row. The layer is selected when the row has a black background. Holding the <shift> key down whilst selecting another layer causes all layers between the first selected layer and the new selection to also be selected.

Zero Offset and Gain

These columns provide linear conversion of the signal values. The diagram shows the nature of the conversion.



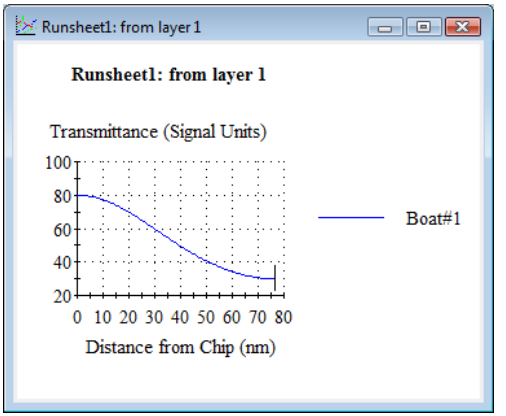
We can write the expression for the conversion as

$$S_{corr} = Gain \times S_{uncorr} - Offset$$

Note that a *positive offset* moves the corrected signal *downwards*, that is towards zero if the signal is positive.

As an example we can look at the first layer of the design in the example below. The total excursion of the signal is 24.4579%. A gain of 2.044 will convert this to an excursion of 50% but the starting signal will move to 188.034%. To make the signal start at 80%, say, we need an offset of 108.034. Putting these figures into the Runsheet yields the following curve for the first layer. The excursion is now 50% as required.

This control reproduces the effect of the corresponding controls on a deposition monitor. It is useful only if the monitor controls are well calibrated.



In addition to entering actual gain and zero offset values, you can enter desired signal values and Runsheet will calculate the required gain and zero offset values for you. There are two modes for gain and zero offset calculations: **Set Gain from One Point** and **Set Gain from Two Points**. These modes are set in the **Edit** menu.

When the mode is Set Gain from One Point, the zero offset is always zero and the gain can be determined from a single point. To calculate a gain, Select Calculate from the Runsheet menu. After the signal values have been calculated, choose a signal value that you wish to define. You may choose any non-blank signal value in the columns: Start At, First Maximum, First Minimum, Last Maximum, Last Minimum or Finish At. In the appropriate cell, type in the signal value that you wish to have and then press <Enter>. The gain for that layer will be adjusted to give the desired signal value. If you wish to apply the gain and zero offset to other layers, click the right mouse button when the mouse is over the layer. A popup menu will appear which has the command apply gain and a sub-menu. The sub-menu allows you to copy the zero offset and gain to all layers on the same chip, all layers in the Runsheet or selected layers.

When the mode is Set Gain from Two Points, the zero offset may be non-zero. In this case you need to enter two points to define the zero offset and gain. The two points are selected in the same way as for Set Gain from One Point. When the first point has been selected and a new value has been entered, the background of the cell will change to red to indicate that first point has been entered. When the second point has been entered, the zero offset and gain will be calculated and applied to the layer(s). The second point does not have to be on the same layer or even the same chip as the first point. The Apply Gain popup menu can be used to copy the zero offset and gain values to other layers in the Runsheet.

Zero Offset and Gain are not applied to wideband calculations.

Wavelength Search

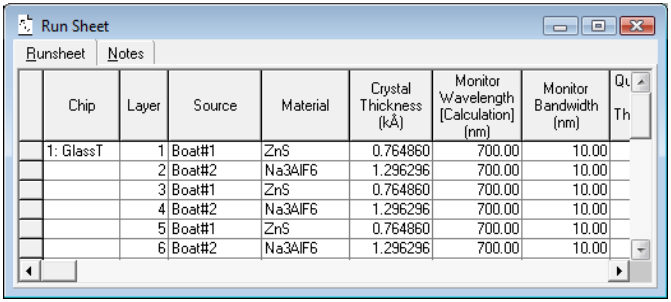
Often the properties of a Runsheet are determined by specifying a monitoring wavelength and bandwidth and then calculating the signal and final swing values. Another approach is to specify a desired final swing value and then determine the monitor wavelength that will give the desired final swing. In Runsheet, the Wavelength Search function provides the ability to find a monitoring wavelength for a layer that will cause termination at a desired final swing.

To use the wavelength search, first enter the desired final swing value into the appropriate final swing cell. Next, with the mouse pointer in the final swing cell, right-click the mouse to display the wavelength search menu. There are two options on this menu: **Find Next Wavelength** and **Find Previous Wavelength**. **Find Next Wavelength** will search for the next monitoring wavelength greater than the current monitoring wavelength that will give the desired final swing value. **Find Previous Wavelength** will search for the next monitoring wavelength less than the current monitoring wavelength that will give the desired final swing value. When the search stops, the Runsheet will be calculated. The displayed final swing value may not be the same as requested, but it will normally be close to the requested value. The difference is controlled by the wavelength search parameters in the Runsheet global defaults (Options menu -> Runsheet)

Exporting a Runsheet

The narrowband data in a Runsheet may be exported to a file in comma separated value format by choosing **CSV file…** from the **Export** sub-menu of the **File** menu. This format is easily imported by spreadsheets for further processing and formatting.

An Example

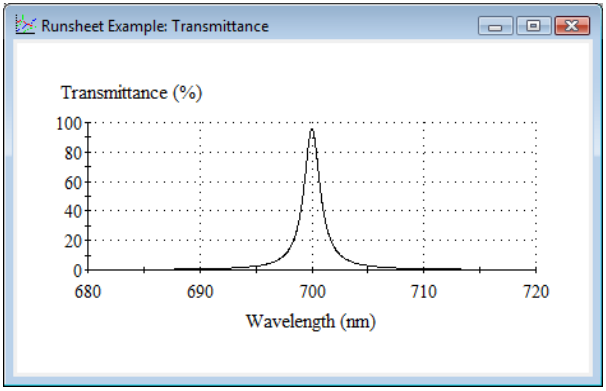


	Chip	Layer	Source	Material	Crystal Thickness (kÅ)	Monitor Wavelength [Calculation] (nm)	Monitor Bandwidth (nm)	Qu Th
	1: GlassT	1	Boat#1	ZnS	0.764860	700.00	10.00	
		2	Boat#2	Na3AlF6	1.296296	700.00	10.00	
		3	Boat#1	ZnS	0.764860	700.00	10.00	
		4	Boat#2	Na3AlF6	1.296296	700.00	10.00	
		5	Boat#1	ZnS	0.764860	700.00	10.00	
		6	Boat#2	Na3AlF6	1.296296	700.00	10.00	

The Runsheet illustrated above carries a design of a single-cavity narrowband filter at 700nm. The design formula is:

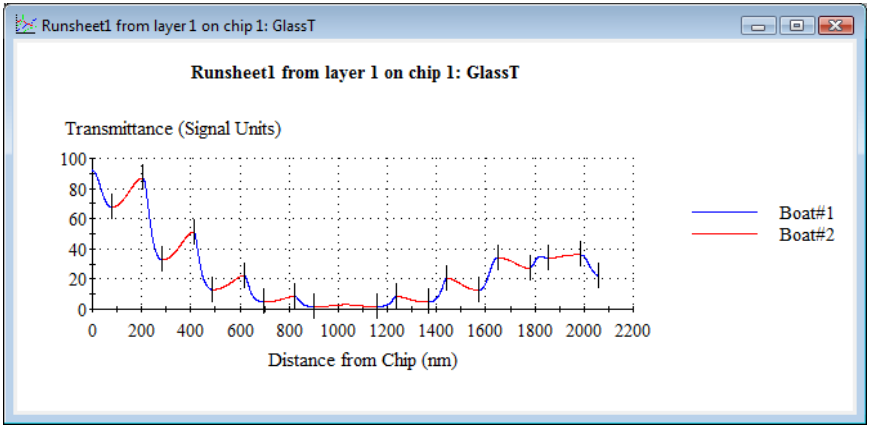
Air | (HL)^5 (LH)^5 | Glass

with Na3AlF6 as low index and ZnS as high index layers. The calculated performance of the filter is shown next.



The default settings in the optical Runsheet are a monitoring wavelength of 700nm with a bandwidth of 10nm. The same glass monitoring chip is used for the entire coating and the optical tooling factors are unity and transmittance monitoring is selected. This, therefore represents direct optical monitoring where the control is exercised on the actual component that is being produced, which is normal for narrowband filter production.

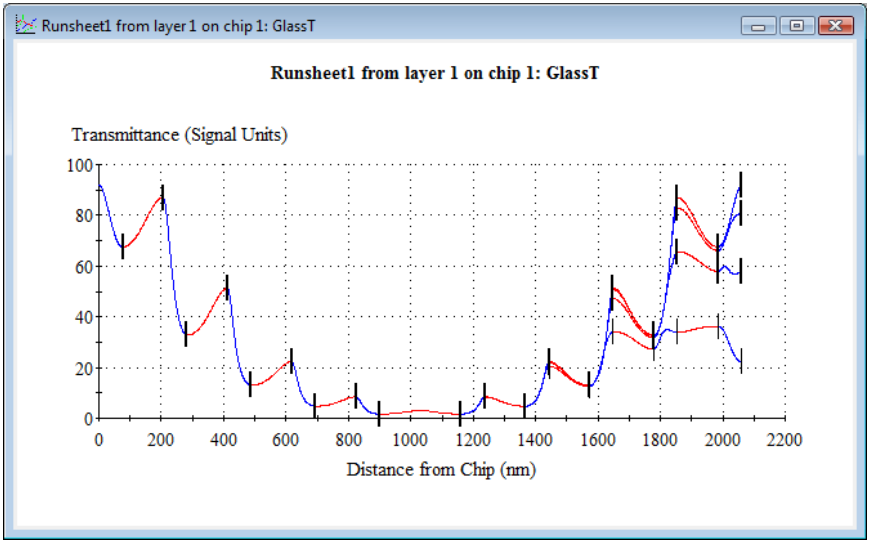
Selecting Plot One Chip from the Runsheet menu produces the plot of the monitoring signal.



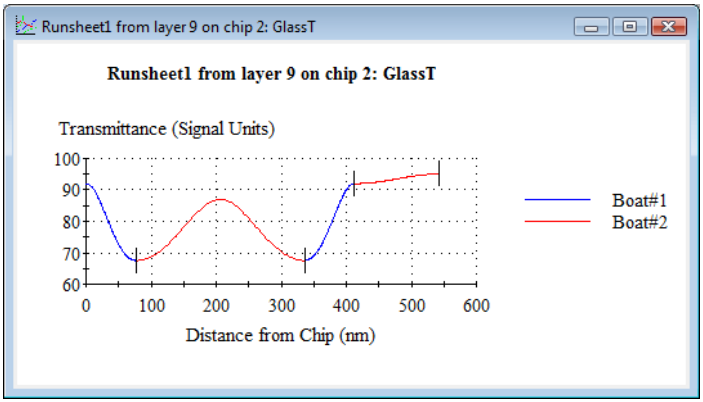
From layer 15 onwards the signal is not at all what should be expected. The problem is the optical bandwidth of the monitoring system. By layer 15 the characteristic curve of the coating is narrower in its spectral features than the monitoring system.

We can vary the monitoring bandwidth and produce a series of curves of gradually decreasing bandwidth to show the effect. Note that the smaller bandwidths use wavelength interval of 1/10th of their width rather than 1nm.

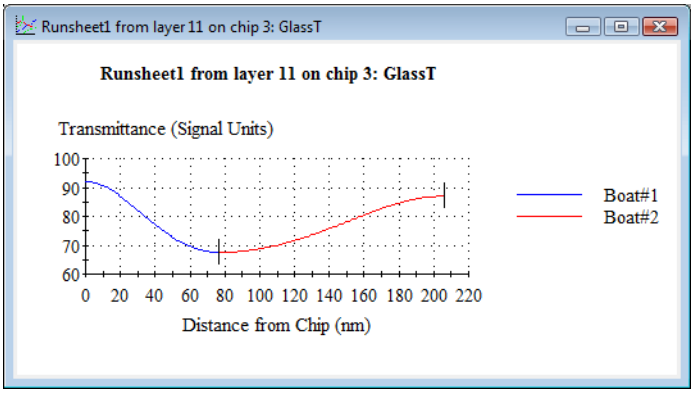
The monitoring system bandwidths from bottom curve to top curve were 10, 3, 1 and 0.1nm. Even the 1nm width shows a falling off of contrast in the final layer although the extremum is in the correct sense and at the correct position. Note the spurious peaks, extremum reversal and lack of contrast. These effects are well known to manufacturers of narrowband filters. But they may also occur in other types of filter.



Monitor chips may be inserted anywhere in the sequence of layers. Each chip is assumed to be fresh and to carry all layers from the point of insertion to the next listed chip. Thus inserting a Glass chip in layers 9 and 13 leads to the following signals.

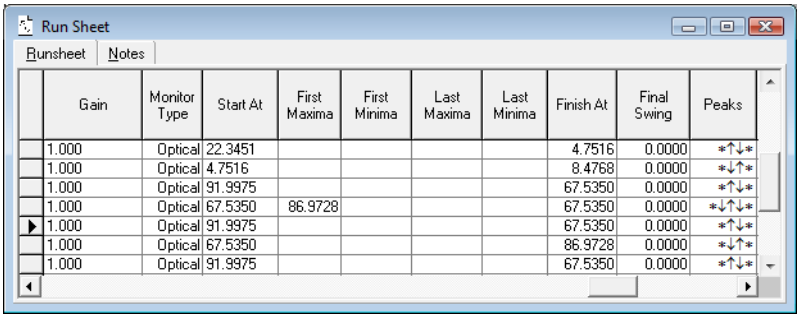


Note that since this starts on an uncoated substrate the contrast in layer 9 (the first in the graph) is larger than in the full coating. Layer 12, though, now may not be giving a very useful signal. We can therefore insert yet another Glass chip at layer 11 and the plot for layers 11 and 12 then becomes as shown.



Selecting Calculate from the Runsheet menu inserts the appropriate values into the Runsheet table. The values listed give information on the starting values, on the terminal values and on the intervening extrema. One column is headed **Final Swing**. Often, absolute values are difficult to obtain in monitoring. The part of the signal between the final extremum and the termination point is therefore compared with the total swing of the coating, expressed as a percentage and listed in the **Final Swing** column. If there is no extremum during the layer then the difference between zero and the starting point is used as a measure of the total swing. The complete sequence for the narrowband filter on one monitoring chip with a monitoring bandwidth of 1nm is shown next. The sheet (shown overleaf) has been scrolled to the extreme right to show the **Peaks** column.

The sequence of extrema in each layer is given in the final column, **Peaks**. Each minimum is denoted by a ↓ and each maximum by a ↑. If a layer starts or finishes at an extremum then it will be listed and also flagged with an asterisk.



	Gain	Monitor Type	Start At	First Maxima	First Minima	Last Maxima	Last Minima	Finish At	Final Swing	Peaks
	1.000	Optical	22.3451					4.7516	0.0000	*↑↓*
	1.000	Optical	4.7516					8.4768	0.0000	*↓↑*
	1.000	Optical	91.9975					67.5350	0.0000	*↑↓*
	1.000	Optical	67.5350	86.9728				67.5350	0.0000	*↓↑↓*
▶	1.000	Optical	91.9975					67.5350	0.0000	*↑↓*
	1.000	Optical	67.5350					86.9728	0.0000	*↓↑*
	1.000	Optical	91.9975					67.5350	0.0000	*↑↓*

For quartz crystal only operation of the Runsheet, the columns that are shown are limited to Layer, Source, Design Material and Crystal Thickness. Calculation is initiated whenever the Runsheet receives either a design file or a machine configuration from the **Edit** menu that completes the set. Again, as in the case of optical monitoring, *the results in the Runsheet are not automatically changed* whenever the design or machine configuration is changed. To change the results a selection from the **Edit** menu must be made even if it is simply a repeat selection of the choice already stated.

Dynamic Tooling Factors

The tooling factor definition is based on a correct design thickness deposited on the batch substrates. The batch thickness is therefore exactly the design thickness. The tooling factor then is defined as the ratio of the rate of deposition on the monitor to the rate of deposition on the batch substrates. A tooling factor less than 1.0 means that less is being deposited on the monitor than on the batch. The Runsheet will always show the monitor signal to give the correct batch thickness.

The tooling factor can be constant or dynamic, that is variable. If it is a constant then throughout the deposition the monitor thickness is building up at a rate that is given by the batch rate times the tooling factor and so the monitor thickness is given simply by the total batch thickness, that is the design thickness, times the tooling factor. For example, a constant tooling factor of 0.5 and a design thickness of 100nm would give a monitor thickness of 50nm.

There are two types of dynamic tooling factor available in the Essential Macleod.

The first type simulates a variable source distribution that can be a depletion effect or, possibly, a variation as it gradually reaches equilibrium. The tooling factor is still the relative rate of deposition but now it is a function of the batch, i.e. design, thickness. The ratio of the actual monitor layer thickness to the batch thickness depends on the way the distribution has varied during the deposition of the complete layer. Since the dynamic tooling factor gives the instantaneous rate, the ratio of the complete thicknesses is given by the integral, or mean, of the dynamic tooling factor over the thickness interval concerned.

The second is a simpler concept where a separate tooling factor applies to each layer in the design. It is described at the end of this section.

Both these tooling factors are defined in a table subject to certain conventions that permit the Runsheet to identify the nature of the data. We begin by considering the first type of dynamic tooling factor associated with source depletion or stabilization.

The dynamic tooling factor is defined in the table with the convention that the factor is constant beyond the upper and lower limits of thickness expressed in the table. It is assumed to be a linear function in between the values that are listed.

If the cumulative thickness is used to derive the values for the tooling factor then it can represent source depletion because successive layers all deposited from the same source move further and further along the curve of tooling factor against thickness. However, it is also possible that the source is permitted to cool between layers and the variation in factor is really due to a gradual reaching of equilibrium of the source through the thickness of the individual layer only. Either of these possibilities for dynamic tooling factor can be set up in the machine configuration.

To set up a dynamic tooling factor the information must first be placed in a table. Use the **New** command from the **File** menu to create a new table. The program will ask how many columns are required. If it is simply a crystal tooling factor or an optical one then 2 columns would be correct. If both crystal and optical factors are to be included in the same file then 3 columns should be chosen. A new table will appear with the required number of columns. Next the nature of the columns must be established. Under the **Edit** menu choose **Columns**. A dialog box appears. Here the most important parameter is Type. For column 1 choose thickness as type and, although not strictly necessary, it is useful to use Thickness also as the heading. Format can also be chosen if desired. See the description earlier or the help file for a description of the various format instructions. (Briefly the format will be similar to ##0.000 or 0.0000E+00 where 0 indicates a digit that must be present and # one that is only present if the number has a digit in that position.) Use Next to move to the second column. Here choose Crystal Tooling Factor or Optical Tooling Factor, as appropriate, as type. This permits the machine configuration to recognize the data as of the correct kind. Once the columns are prepared the data may be entered in the usual way. Remember that table files are eventually set to Read Only when saved. If you must reedit data later remember to reset the Read Only status in the **Edit** menu otherwise *although changes may appear to be made they will not be registered*. The tooling factor file can be saved using any appropriate name and that of the particular material should be quite appropriate. The extension for the file will be **.tbl** because it is a regular table file and it can be plotted in the normal way if required.

The data may need to be converted before entry. Note that it is the instantaneous ratio of deposition rates that is to be stored in the table, that is the dynamic tooling factor. If the existing data refers to total layer thicknesses then they must be converted. This is straightforward. Let us assume that we have the results of a series of tests where different thicknesses were deposited, each starting afresh with a full source and we assume that the changes are sufficiently slow for a linear law to be appropriate for the tooling factor variation in between the data points. We represent the design thicknesses by a_1, a_2 ... and the monitor thicknesses as T_1, T_2 ... Then if f_1, f_2 ... are the dynamic factors we have:

$$T_1 = f_1 a_1$$
$$T_2 = T_1 + 0.5(a_2 - a_1)(f_1 + f_2)$$
$$T_3 = T_2 + 0.5(a_3 - a_2)(f_2 + f_3)$$

These equations can readily be solved to give:

$$f_1 = \frac{T_1}{a_1}$$
$$f_2 = \frac{2(T_2 - T_1)}{(a_2 - a_1)} f_1$$
$$f_3 = \frac{2(T_3 - T_2)}{(a_3 - a_2)} f_2$$

and so on. Essentially, we differentiate the curve of monitor against batch thicknesses. Now we need to set up a machine configuration that will include the factors.

The **New** command in the **File** menu sets up a blank machine configuration for us. This can either be quartz crystal or optical or both. Assume for the moment quartz crystal. The sources must be numbered and assigned a material. Then there is the column, Crystal Tooling Factor. This can either be a number or a file name. For a number, click once in the column cell to activate it and enter the factor. For a file, make sure that the cell is not active by clicking elsewhere if necessary, and then double-click in it. A selection box for the appropriate file will appear. Next we must decide whether or not the dynamic tooling factors should be on the basis of the cumulative thickness that has been deposited - source depletion - or should be applied to each layer independently - source stabilization. There is a check box in the first tab of the machine configuration form labeled **Reset for each Layer**. If this box is unchecked we have the cumulative case. If the box is checked each layer is treated independently. This setting applies to all sources that use dynamic tooling factors.

Finally save the machine configuration under an appropriate name. Note that the program will check for a valid tooling factor by examining the column types as the file is saved and will display an error message if a correct column does not exist.

Let us emphasize once again that the tooling factor tables are intended to represent the *instantaneous* distribution from the source, i.e. what the source is doing at a particular instant rather than the sum total of what it has done from the beginning. Thus the total thickness of a layer is given by the integral of the dynamic tooling factor as a function of theoretical thickness. The reason we have adopted this technique is mainly because it is closer to the physical behavior of the system. A source that reaches a stable distribution, for example, will be represented by a stable tooling factor. This would not be the case if the integral of the tooling factor were used. It is much easier to see whether a proposed table appears realistic when dynamic factors rather than their integrals are used.

The points in the table are linearly interpolated. The tooling factors beyond the final one and before the first one are assumed to be constant.

The alternative type of dynamic tooling factor simply specifies the tooling factor to be used for each layer deposited by a source. To use this new tooling factor type, create a 2 column table. The first column is the layer number and the second column is the tooling factor to be used for that layer. The type of the first column must be set to “Layer Number” and the type of the second column must be either “Optical Tooling Factor” or “Crystal Tooling Factor”. See earlier in this section for more information on creating tooling factor tables. Setting the first column type to “Layer Number” means that the tooling factor will be selected according to layer number, and does not depend on the Dynamic Tooling Convention setting. Instantaneous or Absolute tooling factor tables can be used together with Layer Number tooling factor tables in the same Machine Configuration.

Spectral Weight Data

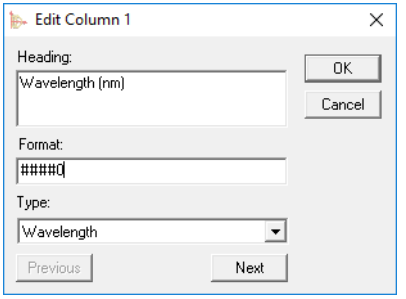
An optical monitoring source for Runsheet may be defined in two ways. It can either be specified as a center wavelength and bandwidth using the **Monitor Wavelength** and **Monitor Bandwidth** columns, or it can be specified using a spectral weight file using the **Monitor Spectrum** column.

A spectral weight file is a table of wavelengths and weight values. The weight values define the relative system response at the corresponding wavelength. The total response is determined by calculating the signal level at each wavelength and then multiplying this value by the weight. The resulting values are then summed and normalized such that the signal with no monitoring chip or layers present will be 100%.

Defining the Spectral Weight Table

To create a table, select **Table** from the **New** sub-menu of the **File** menu. You will be asked to specify the number of columns required. This will normally be two, one for the wavelength and one for the spectral weight. Clicking OK will display a blank table with the requested number of columns.

Next define the titles and content of each of the columns of the table. This is done with the **Edit Columns** option in the **Edit** menu.



A column is defined by three parameters: **Heading**, **Format**, and **Type**. **Heading** is the text that will be displayed as the column header, **Format** is used to format the values in each row of the column and **Type** defines the data that is in the column. For the varying

parameter tables, the type must be correctly defined. The **Previous** and **Next** buttons are used to move to the other columns in the table. The first column must be of type Wavelength and the column containing the weight data (usually the second column) must be of type Spectral Weight. You may use any values you like for the Heading and Format (see the Table Window chapter for more information). Once the columns have been defined, you can enter the wavelength values and weights in the table and then save it.

To instruct Runsheet to use the spectral weight file, double-click in the Monitor Spectrum cell. This will cause a file chooser to be displayed. Select the spectral weight file and then click OK. The units of wavelength in the spectral weight must also be defined. All spectral weight files used in a single Runsheet must have the same wavelength units. These units are defined by the Wavelength Scale Factor command in the Edit menu of the Runsheet. The scale factor is the relationship of the spectral weight wavelength unit to one metre. For example, if the spectral weight wavelength units are in nanometres, then the scale factor is 1E-9. You may use several different spectral weight files in a single Runsheet and you may also mix spectral weight files with Monitor Wavelength/Bandwidth definitions.

Active Plot

Runsheet supports a specialized form of the Active Plot window (see the Active Plot chapter). Runsheet's Active Plot is customized for runsheet data and so has a different set of parameters available. The general concept is the same as for designs: changing the value of a parameter updates the plot with the new signal data.

The Active Plot is started by selecting one of the active plot options from the Runsheet menu: Active Plot One Chip, Active Plot All Chips and Active Plot Selected Layers. These options correspond to the regular plot options in the Runsheet menu. As for the Design Active Plot, parameters must be added to the Active Plot before changes can be made and this is achieved using the Add menu.

Add Menu

This menu contains all the options for adding variables to the Active Plot window. Variables are always added to the end of the existing variables.

Selected Monitor Wavelengths

Adds Monitor Wavelength variables for each of the selected rows in the Runsheet.

All Monitor Wavelengths

Adds Monitor Wavelength variables for all rows in the Runsheet.

Selected Monitor Bandwidths

Adds Monitor Bandwidth variables for each of the selected rows in the Runsheet.

All Monitor Bandwidths

Adds Monitor Bandwidth variables for all rows in the Runsheet.

Selected Tooling Factors

Adds Tooling Factor variables for each of the selected rows in the Runsheet.

All Tooling Factors

Adds Tooling Factor variables for all rows in the Runsheet.

Active Menu

Freeze

The Freeze command saves the current plot curves and starts a new set of curves the next time a variable changes value.

Update Runsheet

This command updates the design in the Runsheet window with the runsheet that has the performance shown in the Active Plot window.

Copy Runsheet

This command copies the runsheet that has the performance shown in the Active Plot window to the clipboard.

The Update and Copy commands do not save any tooling factor changes, since the tooling factors are contained within the Machine Configuration file and not the Runsheet.

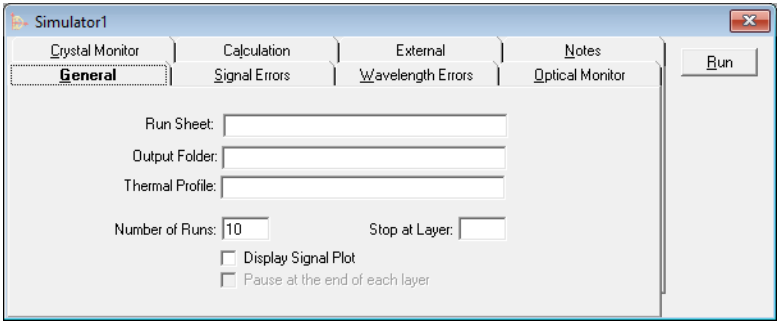
SIMULATOR

The Simulator enhancement to the Essential Macleod has the capability of modeling the behavior of optical and crystal monitoring. This capability is provided by the **Simulator** command in the **New** sub-menu of the Essential Macleod. The **New** sub-menu may be found by clicking on the **File** menu.

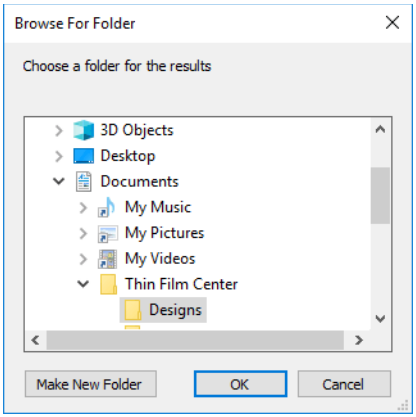
To use the Simulator you must have already produced and saved a calculated Runsheet. Also the design and machine configuration used by the Runsheet must still be present.

General Page

After selecting the **Simulator** option from the **New** menu, the Simulator form will be displayed. The form is split into several tabbed pages that deal with different aspects of setting up the monitor model. The first page that is displayed is the General page.



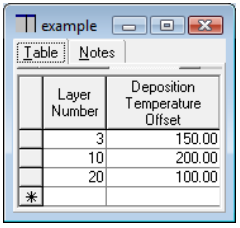
When the model is **Run**, the program will create a number of designs, one for each run, and will place the designs in the folder designated by the **Output Folder** box. Typically the **Output Folder** will specify a new folder that will be created if necessary by the program. If the **Output Folder** exists and contains designs, the designs may be overwritten by the Simulator. The Simulator creates designs with names “1.dds”, “2.dds”, “3.dds”, and so on up to the number of runs specified. Existing files with these names will be overwritten. Double-clicking in the **Output Folder** will display a folder chooser.



With the folder chooser, you can choose an existing folder or create a new folder by clicking **Make New Folder**. After selecting the folder, click **OK** and the path will be entered into the **Output Folder** box. You can also add a new folder name to the text in the **Output Folder** box. It is also possible to type a complete folder path into the **Output Folder** box without using the folder chooser.

The model also needs to have a Runsheet that specifies how the design is to be made. This is contained in a calculated Runsheet. The **Run sheet** box is used to specify the Runsheet file to be used. You can either enter the Runsheet file name directly by typing the path into the **Run sheet** box, or you can double-click in the **Run sheet** box to display a Windows open file dialog. This can be used to select the file and enter it into the **Run sheet** box.

The **Thermal Profile** specifies a temperature profile to be used during the simulation. This may either be a constant temperature offset or it may vary as a function of layer number. For a constant temperature offset, enter the offset in degrees Kelvin. The offset may be positive or negative. For profiles that vary as a function of layer number, a table must first be created that specifies the variation of temperature offset. The table must contain at least two columns. The first column in the table must specify layer number and another column must specify the temperature at the given layer number. The heading for this column must be set to “Deposition Temperature Offset”. Other columns may be present in the table.



An example profile is shown above. Temperature offsets need not be specified for all layers. For layers in between specified layers, the temperature will be linearly

interpolated from the data in the specified layers. Layers before the first specified layer will be deposited at the temperature of the first specified layer and layers after the last specified layer will be deposited at the temperature of the last specified layer. Layers are numbered from the substrate with the layer next to the substrate being numbered 1. Once the table has been created and saved, double-click in the Thermal Profile box. A file chooser will be displayed. Select the table file and then click Open. You can also type the path to the table file directly into the Thermal Profile box.

The **Number of Runs** box specifies how many different simulated deposition runs will be made. A successful model run will produce this number of designs in the **Output Folder**.

If a valid layer number (layer number 1 is next to the substrate) is entered into **Stop at Layer**, then the simulation will pause at the specified layer number.

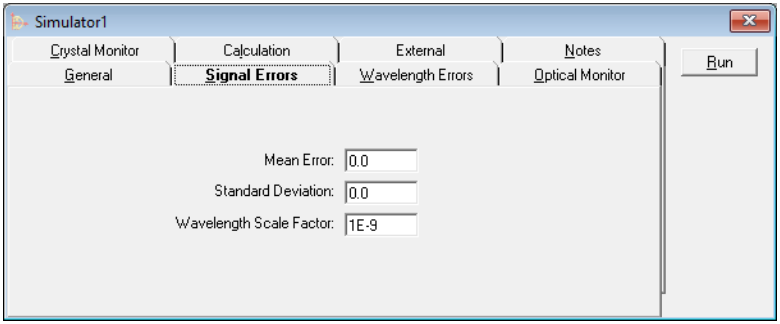
If **Display Signal Plot** is checked, then a stripchart-like display will be presented showing signal variation against time. The production of this display takes a significant amount of the computer's time and is probably best used only to check that the design is being "deposited" correctly. If **Display Signal Plot** is not checked, then the display will still appear, but it will not be updated in as much detail by the computer.

When Display Signal Plot is checked, you can check or clear **Pause at the end of each layer**. When checked, the Simulator will stop at the end of each layer and wait for you to press the **Continue** button on the Simulator run form (see below). You can also toggle layer pausing on the Simulator run form.

The **Run** button is used to start the monitoring process.

Signal Errors Page

The Signal Errors page allows the specification of errors in the signal measurement by a mean and standard deviation. These errors are applied to the calculated signal before the signal is used by the optical monitor part of the model.



For each signal measurement, an error value is randomly selected from a population with a mean and standard deviation. The mean and standard deviation may either be constant or they may vary as a function of wavelength. If the error value lies outside two standard deviations from the mean, then another error value is selected until it lies within two standard deviations of the mean. (The two standard deviation limit applies to all

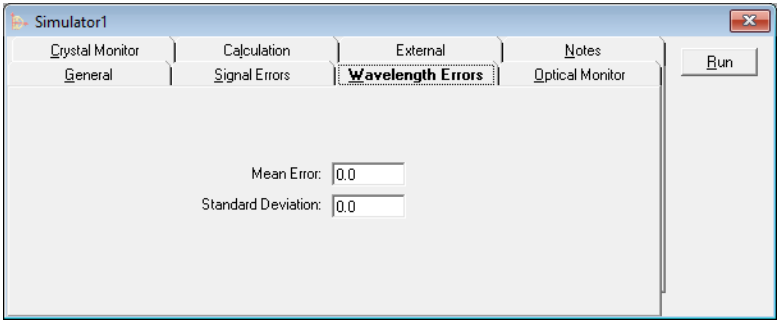
random number selections in the Simulator). After selection, the random number is added to the calculated signal value to provide the value to be used by the monitoring process. The error parameters are expressed in terms of absolute transmittance or reflectance in units of percent (%).

For constant mean or standard deviation, the value is simply entered into the appropriate text box. Where the mean or standard deviation varies as a function of wavelength, the variation is defined in a table (see Defining Varying Parameter Tables) and the filename of the table is entered into the text box. The filename may either be typed directly into the text box, or you can double-click in the text box. This will cause a file chooser to be displayed. Select the file with the chooser and then click OK. This will store the filename in the text box.

Where a table has been specified for either the mean or standard deviation, the Wavelength Scale Factor for the wavelength column must be specified. The Wavelength Scale Factor relates the units of wavelength in the table to 1 metre. For example if the units in the table are nanometres, then the Wavelength Scale Factor is 1E-9. If tables are used for both mean and standard deviation, then the wavelength units must be the same. This is most easily achieved by specifying the mean and standard deviation in the same table.

Wavelength Errors Page

The Wavelength Errors page allows the specification of errors in wavelength setting by a mean and standard deviation.



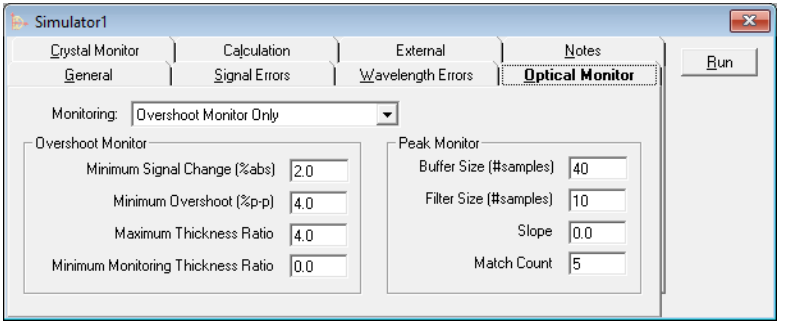
A wavelength error value is generated in the same way as a signal error value is generated each time a new wavelength is set. The model assumes that once a wavelength is set, it does not change. The wavelength error is added to the desired wavelength to result in an actual wavelength used for measurement. The units of wavelength are always nanometres. Errors in bandwidth are assumed to never occur. Mean and Standard Deviation for wavelength errors may only have constant values.

The wavelength setting errors are not applicable where a spectral weight file has been used to define the light source in Runsheet. If you wish to model the performance of an optical monitor with a known source spectrum such as the output of a source lamp and narrowband filter, or model the output of a monochromator which has harmonic and other leaks, then a spectral weight file can be used to describe the spectrum used in the

monitoring process. The spectral weight file to be used is specified in the Runsheet. If a spectral weight file was specified for the Runsheet calculations (in the **Monitor Spectrum** column) and no spectral weight file was specified for simulation, then the Monitor Spectrum file will be used for the simulation. Where a file for use in simulation has been specified (in the **Simulation Spectrum** column) then this file will be used for the simulation. See Defining Varying Parameter Tables for information on defining spectral weight files.

Optical Monitor Parameters Page

The Optical Monitor Parameters page contains parameters that control how the optical monitor model recognizes peaks and troughs in the monitoring signal.



Simulator provides two kinds of optical monitor: An overshoot monitor and a peak monitor. The overshoot monitor is designed for monitoring non-quarterwave designs where layers are not cut at an extremum. The peak monitor is designed to cut at extrema and so is only appropriate for quarterwave type designs.

Overshoot Optical Monitor

The overshoot optical monitor operates by counting peaks regardless of their sign. After the required number of peaks have been counted, the monitor will stop deposition as soon as the signal reaches the specified (in the Runsheet) proportion of the last seen peak to peak excursion. In order to detect a peak, the model must see the signal move to an extremum and then move away. A peak is recognized when signal has moved away from the peak by the **Minimum Overshoot** proportion.

To reduce the probability of recognizing false peaks caused by signal noise, the **Minimum Signal Change** parameter specifies a minimum absolute signal change that must occur before peak recognition is enabled. This minimum value is applied to signal changes as the signal moves towards the extremum and signal changes as the signal moves away from the extremum.

The **Maximum Thickness Ratio** parameter prevents Simulator from indefinitely depositing material in conditions where the overshoot monitor will never terminate a layer. This may happen, for example, when the peak-to-peak signal variation is less than the Minimum Overshoot value. Once Simulator has deposited (Maximum Thickness

Ratio * design layer thickness), Simulator will cut the layer regardless of the state of the overshoot monitor.

The **Minimum Monitoring Thickness Ratio** specifies the thickness at which the optical monitor will start monitoring. The thickness at which monitoring will start is given by the ratio value * the design layer thickness or the ratio value * the thickness of one quarterwave which ever is the smaller. This value is used to prevent the monitor from recognizing peaks near the start of a layer that should not be counted.

As an example consider a signal which starts at 45% rises to a peak of 67% and then falls. The minimum signal change is set to 2% and the minimum overshoot is 4%. The Runsheet specifies that the cut should be made at a final swing of 22%. At the start of deposition when the signal is 45%, the peak detection is disabled. When the signal reaches 47% peak detection is enabled. If signal were to fall back below 47%, peak detection would be disabled. As the signal rises to its maximum of 67%, the optical monitor maintains a record of the peak signal seen. As the signal starts to fall, peak detection is temporarily disabled until the signal has fallen by at least 2% (i.e. when it falls below 65%). When signal falls below 65%, the monitor then waits for the signal to fall below the minimum overshoot which is at a signal level of:

$$67 – (67\text{-}45) *0.04 = 66.12\%$$

Since this has already occurred when the 2% minimum signal change has been satisfied, the peak is recognized and logged as soon as the 2% minimum signal change has been met.

If the Runsheet called for a single quarterwave of material to be deposited, the deposition would stop at this point. For the final swing of 22%, the monitor would wait until the signal had fallen to

$$67 – (67\text{-}45)*0.22 = 62.16\%$$

before stopping deposition for the layer.

Peak Optical Monitor

The peak optical monitor operates by sampling the signal data and looks for a zero slope in the signal. The zero slope is detected by comparing the latest signal value with a previous signal value. The peak monitor contains several features to minimize false peak recognition. Firstly the measured signal is passed through a mean filter. The size (in number of samples) of this filter is specified in the **Filter Size (#samples)** parameter. Initially, while the filter is filling up with samples, there will be no output values. Once the filter is full, for each sample read in, the filter will output a value that is the mean of the last filter size of samples read in. Also the oldest sample will be discarded to make room for the next sample. Thus this filter provides a moving average of the input signal data.

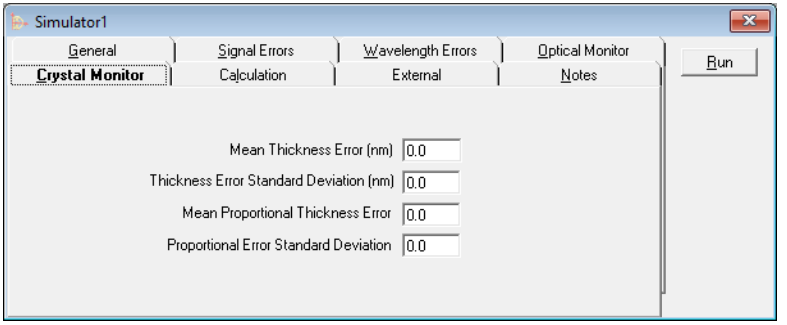
Values generated by the mean filter are entered into a buffer. The size of this buffer is specified in the **Buffer Size (#samples)** parameter. The slope comparison is performed by comparing the oldest entry in the buffer with the newest. This comparison is only performed when the buffer has filled up with samples. Once the buffer has filled up, the oldest sample is discarded to make room for the next sample. The slope (as measured by the difference between the oldest and newest values) is compared to the required Slope

value. When the slope in the buffer has exceeded the required **Slope** a user-specified **Match Count** number of times, the peak is recognized.

To use the Peak Optical monitor, deposition rate data must have been specified in the Machine Configuration file, the **Use Rate Data** box must be checked on the **Calculation** tab, and a **Sampling Rate** must also be defined.

Crystal Monitor Parameters Page

The Crystal Monitor Parameters page controls the errors applied to layers when deposited using the crystal monitor model.



For crystal monitoring, errors on one layer are assumed to be independent of errors present in deposited layers. You can define two sets of parameters for layer errors. The Mean Thickness Error and Thickness Error Standard Deviation are parameters for absolute errors that are independent of thickness. For these parameters the generated random error is added to the final layer thickness to produce the deposited layer thickness.

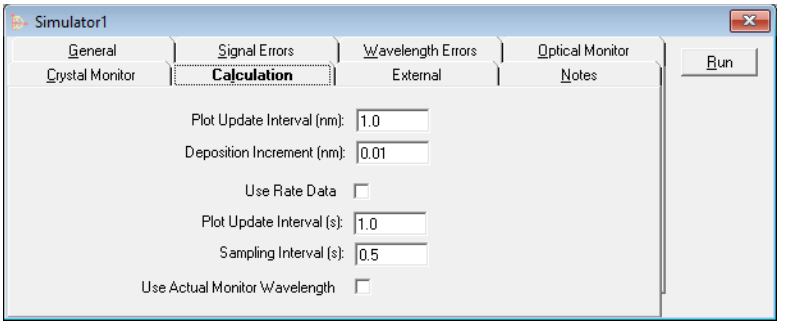
Mean Proportional Thickness Error and Proportional Error Standard Deviation are parameters for proportional errors whose absolute magnitude is defined by the thickness of the layer. For proportional errors, the Layer thickness is modified as follows:

Deposited Layer Thickness = Layer Thickness * (1 + Random Error)

Where both Absolute and Proportional thickness errors have been defined, the Absolute errors are applied first and then the Proportional errors are applied.

Calculation Page

The calculation page provides control over the calculations performed by Simulator.



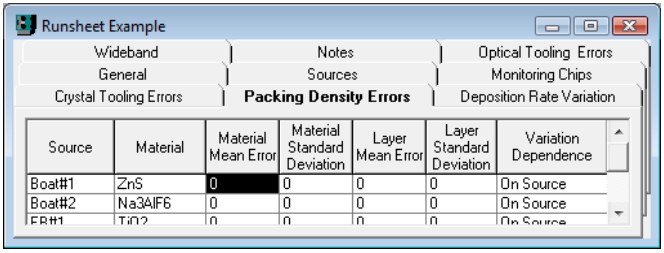
Plot Update Interval controls the rate at which the optical monitor signal plot is updated in terms of thickness of deposited material. Larger values cause the plot to be updated less frequently. This causes the simulation to run faster.

Deposition Increment defines the amount of material that is deposited at each simulation step. Increasing this value will cause the simulation to run faster but at the expense of less accurate deposition results.

The effect of variations in the deposition rate may be examined by defining deposition rate information in the Machine Configuration file (see below) and by checking **Use Rate Data**. When **Use Rate Data** is checked, a sample of the current optical signal will be taken every **Sampling Interval** seconds.

Packing Density Errors

Packing Density Errors have a more complicated specification than Wavelength and Signal Errors. Two error terms may be applied: A material error and a layer error. The material error is generated and applied once for each material for each “deposition” run. The layer error is generated and applied for each layer in each “deposition” run. These two error terms are set for each source and, for this reason, they are defined in the machine configuration.



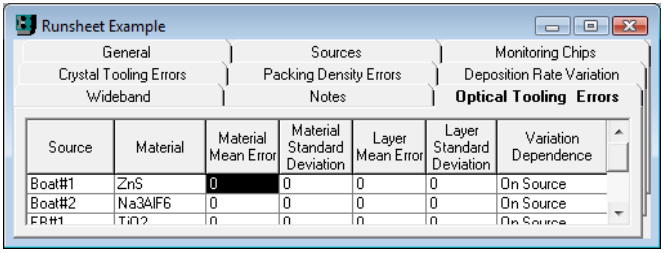
Material Mean Error and Material Standard Deviation specify the parameters for generating the material errors. These values are always constants. The Layer Mean Error and Layer Standard Deviation specify the parameters for generating the Layer Errors. These may either be constant or vary as a function of deposited thickness. The deposited

thickness may either be the thickness deposited from the source (select On Source in the Variation Dependence column), or the thickness deposited from all the sources (select On Total in the Variation Dependence column. The thickness units used for the tables defining the variation of layer parameters are those of the dynamic tooling factor thickness units and are specified on the General tab. For information on defining the tables see Defining Varying Parameter Tables.

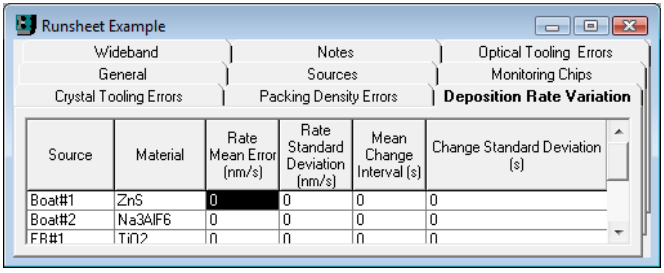
Packing density errors are proportional errors. The packing density of the "deposited" layer is given by (1.0 + M + L) * (actual packing density) where M is the material error and L is the layer error.

Tooling Factor Errors

Tooling Factor Errors are specified and applied in the same way as Packing Density Errors except that they modify the final thickness of the layers and not the packing density. Furthermore, separate tooling factor errors are specified for optical monitoring and for quartz crystal monitoring. These errors are specified in the machine configuration on the Optical Tooling Errors tab and on the Crystal Tooling Errors tab.



Deposition Rate Variation



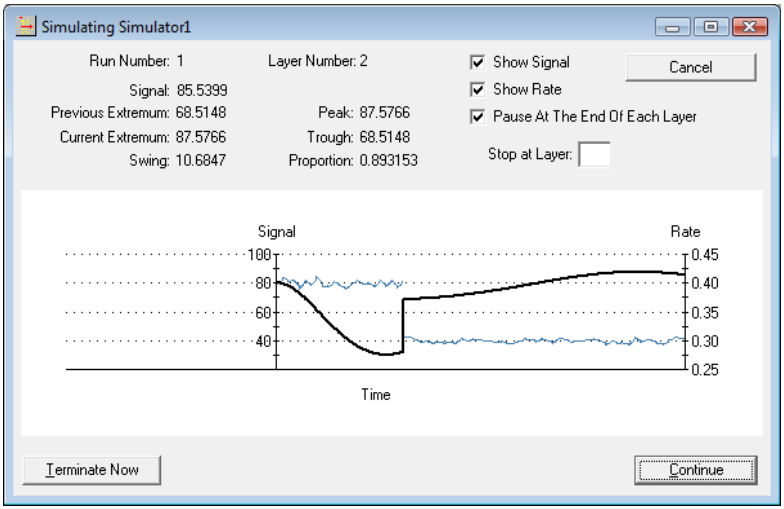
Variations in deposition rate are modeled in the **Deposition Rate Variation** tab of a Machine Configuration. Deposition rates for each source are defined in the **Sources** tab, the **Deposition Rate Variation** tab then specifies, for each source, parameters for varying the rate. The deposition rate varies linearly from one rate to another. At the start of a layer, the deposition rate is given by the deposition rate defined on the Sources tab + an offset given by a random number drawn from a population with a mean given **by Rate**

Mean Error and a standard deviation given by **Rate Standard Deviation**. This rate will change linearly until it reaches a new rate. The new rate is given by the source deposition rate + another offset given by a new random number. The time at which the new rate is reached is given by a random time value drawn from a population with mean **Mean Change Interval** and standard deviation **Change Standard Deviation**.

When the simulation has reached the new rate, another time value is generated and a new rate to be achieved at that time value is also generated. Deposition then continues with the deposition rate linearly varying such that the new rate at the new time is met.

Executing the Model

Once all the model parameters have been established, the model can be executed by clicking the **Run** button. This will show the monitoring progress screen that provides details about the progress of the model.



The monitoring progress screen provides information for layers that are optically monitored. **Signal** shows the instantaneous signal level in the Simulator. **Previous Extremum**, **Current Extremum** and **Swing** show information about the state of the optical monitor. **Current Extremum** shows the value of the most recently recognized extremum. **Previous Extremum** shows the value of the extremum that was recognized before the current extremum. **Swing** indicates the current signal level expressed as a percentage of the range between **Previous Extremum** and **Current Extremum** i.e.

$$Swing = 100\frac{Signal - Current\ Extremum}{Previous\ Extremum - Current\ Extremum}$$

Peak, **Trough** and **Proportion** provide information about the recent history of the monitoring signal. **Peak** is the highest signal value seen since the last **Trough**. **Trough** is the lowest signal value seen since the last **Peak**. **Proportion** is the current signal level expressed as a proportion of the **Peak** to **Trough** range.

The **Show Signal** checkbox turns the signal plot and information on and off. Turning the display off causes the simulation to run faster at the expense of not being able to see the signal variation during layer deposition. When deposition rate is being used, the **Show Rate** checkbox controls the display of deposition rate information.

Cancel stops the simulation and returns you to the Simulator parameters window. Any runs that have been completed will be saved and are available for analysis.

Pause At The End Of Each Layer toggles between continuous simulation and stopping at the end of each layer. When **Pause At The End Of Each Layer** is checked, the simulation will stop at the end of each layer. Press the **Continue** button to continue the simulation.

To pause simulation at a particular layer, enter the layer number into the **Stop at Layer** box. When Simulator reaches the layer, it will stop deposition and await the next command.

Terminate Now allows you to force termination of a layer at the point when you click the button. This can be used to simulate a manual monitoring technique or to force the simulation to move on to the next layer because the optical monitor has not correctly recognized the end of a layer.

After Simulator has completed, the performance of all of the designs produced can be displayed by selecting Plot from the Performance menu. The Parameters menu allows you to alter the performance parameter that is calculated. All the designs produced by Simulator are stored in the Output Folder. The designs can be individually opened and examined.

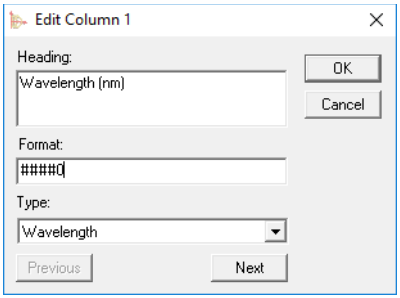
Defining Varying Parameter Tables

Many of the parameters that can be defined in Simulator can be expressed as function of some independent variable as well as having a constant value. These functions are defined by creating a table and entering data values. The table is then saved and the file name is entered into the appropriate text box on the Simulator parameters form. Tables may also be specified in a Machine Configuration and a Runsheet.

Where varying parameters can share a common independent variable such as mean and standard deviation, they can be defined in a single table. A type indicator is used to define the data that is contained in each column of the table.

To create a table, select **Table** from the **New** sub-menu of the **File** menu. You will be asked to specify the number of columns required. This should be the number of dependent variables required plus one for the independent variable. Clicking OK will display a blank table with the requested number of columns.

Next define the titles and content of each of the columns of the table. This is done with the **Edit Columns** option in the **Edit** menu.



A column is defined by three parameters: **Heading**, **Format**, and **Type**. **Heading** is the text that will be displayed as the column header, **Format** is used to format the values in each row of the column and **Type** defines the data that is in the column. For the varying parameter tables, the type must be correctly defined. The **Previous** and **Next** buttons are used to move to the other columns in the table.

The independent variable in a varying parameter table must always be in the leftmost column. This is usually of type Wavelength or Thickness. The dependent variables may be in any of the remaining columns and must have their types correctly set.

The following table lists the Simulation parameters, the corresponding table column types and the independent variable type.

Simulation Parameter	Table Column Type	Independent Variable Type
Signal Mean Error[1]	Signal Mean Error	Wavelength
Signal Standard Deviation[1]	Signal Standard Deviation	Wavelength
Optical Tooling Factor: Layer Mean Error[2]	Optical Tooling Factor Mean Error	Thickness
Optical Tooling Factor: Layer Standard Deviation[2]	Optical Tooling Factor Standard Deviation	Thickness
Crystal Tooling Factor: Layer Mean Error[2]	Crystal Tooling Factor Mean Error	Thickness
Crystal Tooling Factor: Layer Standard Deviation[2]	Crystal Tooling Factor Standard Deviation	Thickness
Packing Density: Layer Mean Error[2]	Packing Density Mean Error	Thickness
Packing Density: Layer Standard Deviation[2]	Packing Density Standard Deviation	Thickness
Monitor Spectrum[3]	Spectral Weight	Wavelength

Simulation Spectrum[3]	Spectral Weight	Wavelength

1) This parameter is found in Simulator

2) This parameter is found in Machine Configuration

3) This parameter is found in Runsheet

Once the columns have been defined, the values may be entered by typing values into the cells of the table. Complete tables may also be pasted in from the clipboard.

External Tab: Altering the Monitoring Algorithm

When the enhancements Simulator and Function are both enabled, a script can be written that provides the monitoring algorithm to be used by Simulator. Script support is provided for narrow-band and wide-band optical monitoring. Layers monitored by crystal do not use scripts. When a script is used with Simulator, the script implements various functions that will be called by Simulator during execution of the simulation. As each function is called, various variables will contain updated values of simulation parameters. These values are to be used by the monitoring algorithm in the script as necessary. The script also has access to the Simulator data and through the Simulator object, the Runsheet data, the Machine Configuration data, the Design data and Materials data.

The Browse button in the External Tab of Simulator accesses the Scripts folder and permits entry of the monitoring script name in the Monitor Script field. Full instructions on preparing the script and using it with Simulator are in the Scripting Manual that is contained in the Help Manual.

DWDM ASSISTANT

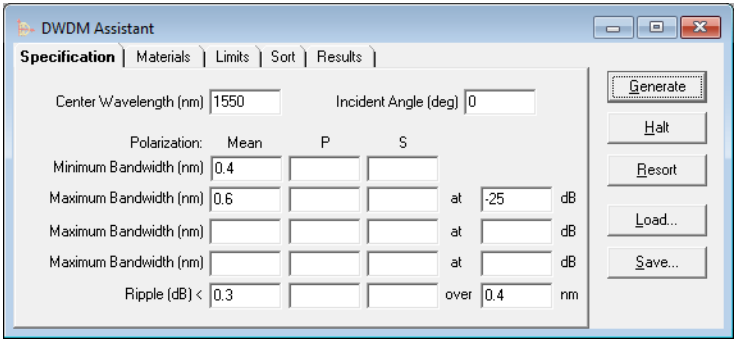
The DWDM Assistant designs bandpass filters using the method of symmetrical periods. The DWDM Assistant is started by clicking on **DWDM Assistant** in the **Tools** menu.

The DWDM Assistant is organized as a series of tabbed pages. The first four pages are used to enter the specification of the bandpass filter and to provide constraints on the design process. Once all the information has been entered, you click the Generate button. The DWDM Assistant then starts the process of designing the filters. Properties of the generated designs are displayed in the last tabbed page. A particular design can be examined in detail by double-clicking on the desired row in the Results page.

The DWDM Assistant limits itself to the design of the quarterwave layers in the filter. Often a simple anti-reflection coating is applied to the front of the coating or to the substrate before the quarterwave layers are deposited. This anti-reflection coating is easily designed by using refinement to adjust the thicknesses of the anti-reflection coating layers to give the best transmittance.

Specification Page

After selecting the **DWDM Assistant** option from the **Tools** menu, the DWDM Assistant form will be displayed. The form is split into several tabbed pages that deal with different aspects of setting up design process. The first page that is displayed is the Specification page.

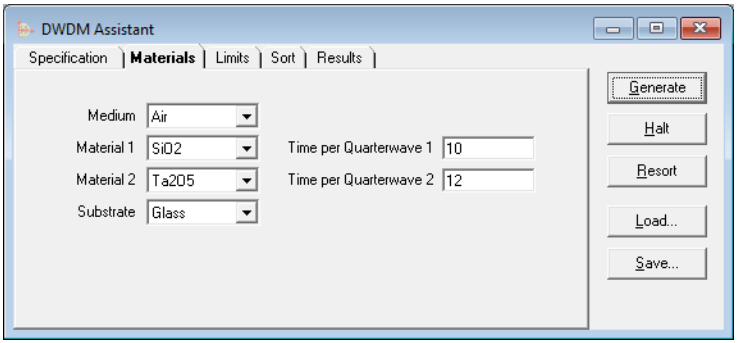


The filter is specified in terms of center wavelength, a minimum bandwidth, up to three maximum bandwidths and a ripple performance. The minimum bandwidth is the bandwidth at the outermost peaks of the filter. In general, a bandwidth specified at a specific transmission level (such as –0.3dB or –0.5dB) will be slightly wider than the minimum bandwidth value. Each maximum bandwidth is specified at a particular transmission level. This allows you to enter specifications with multiple bandwidth limits. If you have less than three maximum bandwidth specifications, the remaining bandwidth specifications should be empty. The ripple specification may be given for a different width than the minimum bandwidth. This allows you to specify a filter with a ripple requirement over a narrower range than the minimum bandwidth. The ripple is

measured as the difference between the highest and lowest transmittance in the ripple bandwidth. The ripple bandwidth is always centered over the center wavelength.

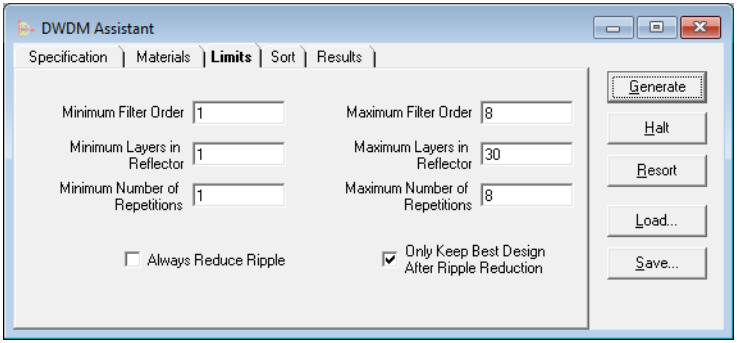
Materials Page

The materials page is used to enter details of the materials to be used in the design. Material 1 and Material 2 specify the thin-film materials to use. It does not matter which box is used to define the high index material or the low index material. Time per Quarterwave 1 and Time per Quarterwave 2 specify the deposition time in arbitrary time units for a quarterwave of material 1 and material 2 respectively. These rates are used to estimate a total deposition time for each candidate design. The results can be sorted based on deposition time (as well as other parameters).



Limits Page

The limits page controls the extent of the search for bandpass filter designs.



The **Minimum Filter Order** and **Maximum Filter Order** control the size of the largest cavities in the bandpass design. The size of a cavity is the filter order multiplied by one half-wave thickness. Cavities may be made from either high index material or low index material.

The **Minimum Layers in Reflector** and **Maximum Layers in Reflector** control the range of the number of layers between each cavity in the filter that form the reflectors either side of the cavity.

The **Minimum Number of Repetitions** and **Maximum Number of Repetitions** control the limits on how much the central symmetrical period may be repeated. The more times the central period is repeated, the steeper the sides of the filter.

A basic filter is constructed by repeating a central period a certain number of times and then providing matching structures to match the central period to the substrate and to the medium. This basic design may be sufficient to meet the ripple specification. If **Always Reduce Ripple** is not checked, then this design will be entered into the results table as a candidate design. If **Always Reduce Ripple** is checked, then regardless of the ripple performance of the design, the DWDM Assistant will always attempt to add extra matching structures to improve the ripple further.

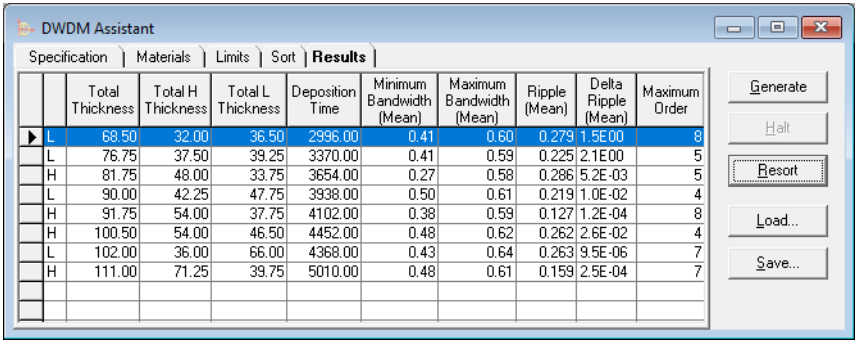
If the DWDM Assistant is adding extra structures to improve the ripple performance, there will, in general, be several structures that improve the ripple sufficiently to meet the ripple specification. If **Only Keep Best Design After Ripple Reduction** is checked then only the best design from the ripple reduction will be kept and entered into the Results page. If **Only Keep Best Design After Ripple Reduction** is not checked, then all designs generated during ripple reduction that meet the ripple specification will be entered into the results page.

Sort Page

The Sort page specifies how the candidate designs are to be sorted on the Results page. Candidate designs may be sorted by up to four parameters. The sort parameter is chosen from the selection offered after **Sort By**. The direction may also be specified. If **Ascending** is selected, then the smallest value of the chosen parameter will be displayed first. If **Descending** is selected, then the largest value of the chosen parameter will be displayed first. The Results page can be re-sorted after generating the designs by altering the Sort page and then clicking **Resort**.

Results Page

The Results page displays all the candidate designs generated by the DWDM Assistant. Once all the parameters have been entered, click **Generate** to start the design process. The Results page will be automatically selected and the DWDM Assistant will enter designs as they are completed. You can stop the design process at any time by clicking the **Halt** button.



	Total Thickness	Total H Thickness	Total L Thickness	Deposition Time	Minimum Bandwidth (Mean)	Maximum Bandwidth (Mean)	Ripple (Mean)	Delta Ripple (Mean)	Maximum Order
L	68.50	32.00	36.50	2996.00	0.41	0.60	0.279	1.5E00	8
L	76.75	37.50	39.25	3370.00	0.41	0.59	0.225	2.1E00	5
H	81.75	48.00	33.75	3654.00	0.27	0.58	0.286	5.2E-03	5
L	90.00	42.25	47.75	3938.00	0.50	0.61	0.219	1.0E-02	4
H	91.75	54.00	37.75	4102.00	0.38	0.59	0.127	1.2E-04	8
H	100.50	54.00	46.50	4452.00	0.48	0.62	0.262	2.6E-02	4
L	102.00	36.00	66.00	4368.00	0.43	0.64	0.263	9.5E-06	7
H	111.00	71.25	39.75	5010.00	0.48	0.61	0.159	2.5E-04	7

The sample results page above shows some candidate designs. The leftmost untitled column shows the index of the main cavities. If H is displayed, then the cavities are made from high index material, and if L is displayed, then the cavities are made from low index material. The Delta Ripple column indicates the sensitivity of the design to a change in tooling factor. The thickness of the L layers is made slightly thicker and the thickness of the H layers is made slightly thinner. The Delta Ripple is the difference between the ripple of this new design and the ripple of the original design. A smaller Delta Ripple indicates a lower sensitivity.

To look at a design in more detail, double-click in the gray selection column of the appropriate row at the left side of the page. This will cause a design to be generated containing the candidate design. The design below was generated by double-clicking on the highlighted row in the above results page.

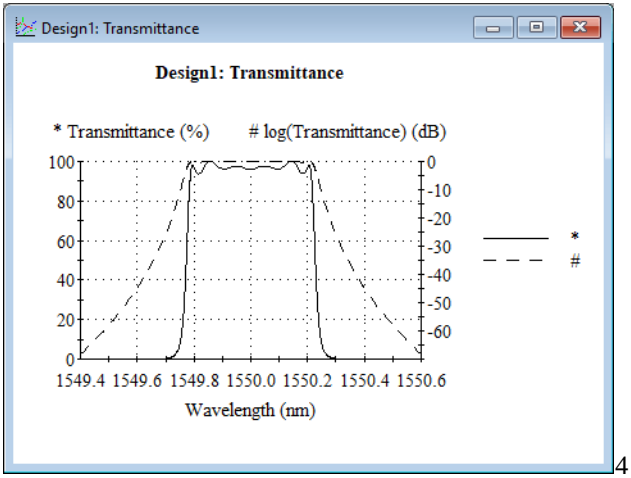
Design1

Design | Context | Notes

Incident Angle (deg)	0.00
Reference Wavelength (nm)	1550.00

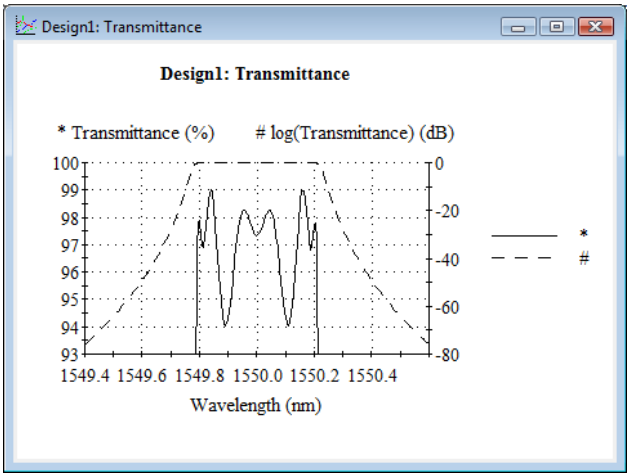
	Layer	Material	Refractive Index	Extinction Coefficient	Optical Thickness (FWOT)	Physical Thickness (nm)
▶	Medium	Air	1.00000	0.00000		
	1	Ta2O5	2.10000	0.00000	0.25000000	184.52
	2	SiO2	1.44402	0.00000	0.25000000	268.35
	3	Ta2O5	2.10000	0.00000	0.25000000	184.52
	4	SiO2	1.44402	0.00000	0.25000000	268.35
	5	Ta2O5	2.10000	0.00000	0.25000000	184.52
	6	SiO2	1.44402	0.00000	0.25000000	268.35
	7	Ta2O5	2.10000	0.00000	0.25000000	184.52
	8	SiO2	1.44402	0.00000	0.25000000	268.35
	9	Ta2O5	2.10000	0.00000	0.25000000	184.52
	10	SiO2	1.44402	0.00000	0.25000000	268.35
	11	Ta2O5	2.10000	0.00000	0.25000000	184.52
	12	SiO2	1.44402	0.00000	0.25000000	268.35
					68.50000000	62797.87

This design has the performance shown below:



4

Zooming in on the performance in the passband, we can see we could improve the overall transmittance by adding an anti-reflection coating to the design.



Candidate designs produced by the DWDM Assistant can be saved by clicking the **Save** button. The candidates may be subsequently restored by clicking the **Load** button.

MONITORLINK for EDDY LMC-10

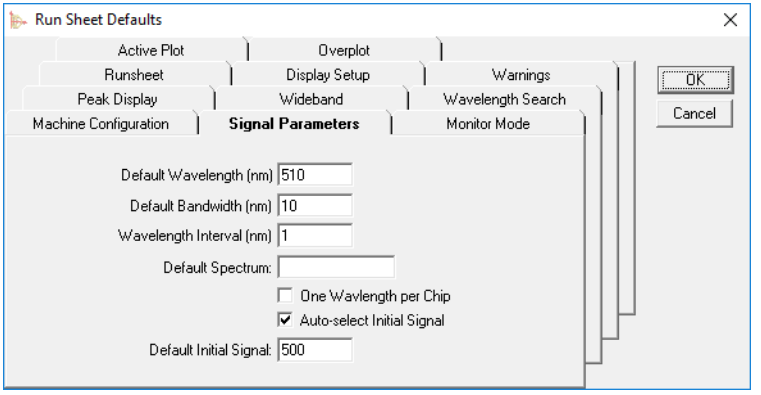
Modifications to Runsheet

Runsheet Defaults

The **Run Sheet…** item in the **Options** menu activates a **Run Sheet Defaults** window with, normally, three tabs. However, in a Runsheet that has been configured by Monitorlink to suit a particular controller there may be an extra tab. The figures below show the regular window followed by that for the Eddy LMC-10 Controller, where there is an extra tab, **Warnings**.

Please note that this description is devoted purely to the features of the enhancement to the Essential Macleod. It is no substitute for the manual for the monitor.

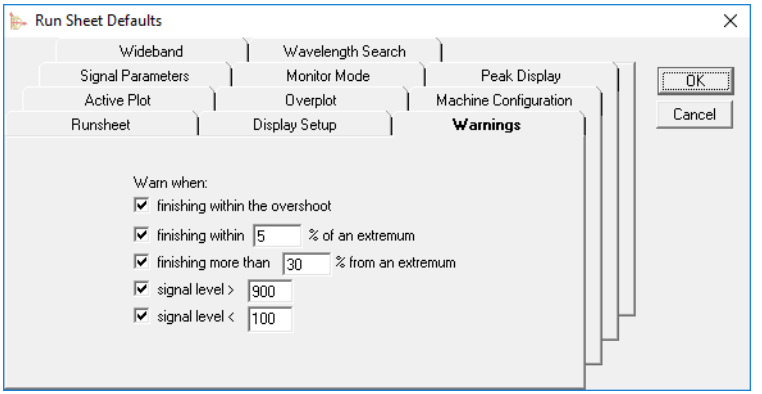
The **Machine Configuration** tab is unchanged.



The **Signal Parameters** tab shows two extra items. The regular Runsheet asks for **Default Wavelength**, **Bandwidth** and **Wavelength Interval**. These are described in the earlier section devoted to Runsheet. The two extra items are **Auto-select Initial Signal** and **Default Initial Signal**. The Eddy LMC-10 operates on the basis of a signal that varies between 0 and 1000 units, preferably between, say, 100 and 900 units. There is no offset and the gain is varied to adjust the signal level. In the mode of operation that yields programs for the Eddy controller, the gain and zero offset columns are therefore suppressed. The Runsheet generator is set automatically to vary the gain with the option either of a given level for the starting signal, or a maximum signal excursion which is determined by making the largest signal coincide with the upper limit. When **Auto-select Initial Signal** is checked, Runsheet maximizes the upper signal level. When **Auto-select Initial Signal** is unchecked the initial signal level is set to coincide with the **Default Initial Signal Level**. In either case, however, adjustments will be made if the signal for at least part of the layer is outside the allowed range.

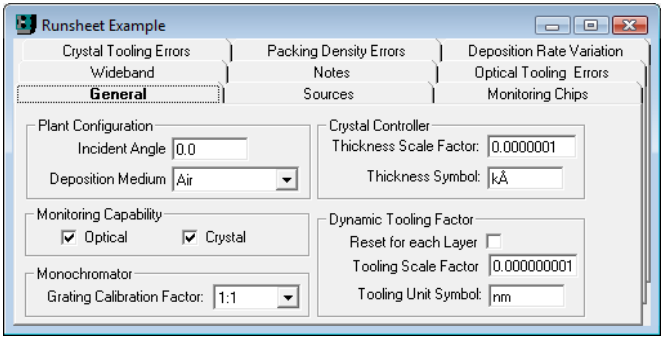
Monitor Mode, the next tab, is simply transmittance or reflectance as before.

Warnings relate to various signal levels and termination conditions. Single-wavelength monitoring processes give best precision when there is an overshoot that is reasonably large but not too large. The default values are simply suggestions. The signal levels shown of 100 and 900 units are chosen to be comfortably within the 0 to 1000 limit of the Eddy LMC-10 Controller so that an unexpectedly large signal excursion can still be accommodated.



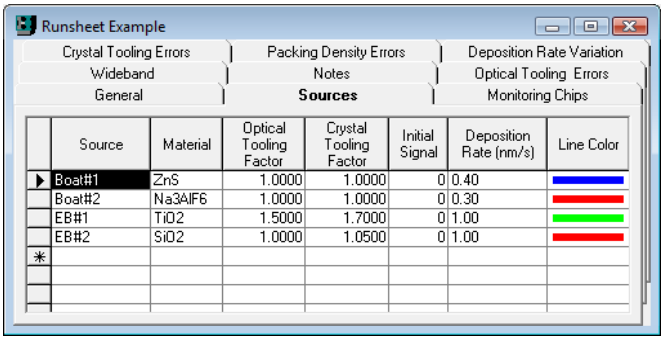
Machine Configuration

There are some additions to the Machine Configuration. The first is in the Edit menu that now has two additional items, **Eddy Machine Configuration** and **Generic Machine Configuration**. The first gives the special form of the configuration for use with the Eddy monitor while the second gives the configuration already described in the Runsheet section of the manual.

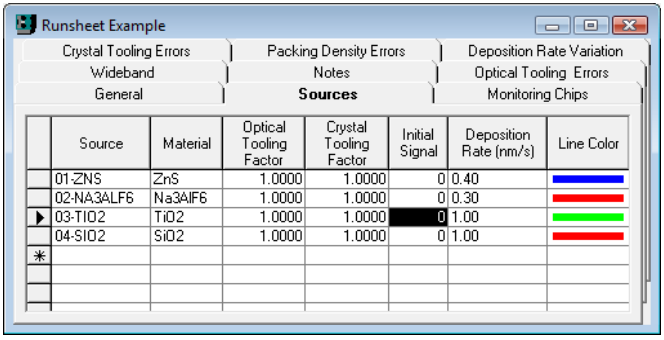


There are two differences in the Eddy version. The first is that a **Grating Calibration Factor** is to be entered. This tells the system the order of diffraction that is being used in the grating monochromator.

Then in the Sources tab there is an extra column, **Initial Signal**. This is an initial signal that is set against each source of material and overrides the global default if entered.



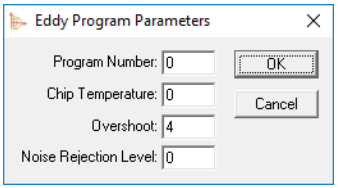
The Edit menu has a new item, **Load Eddy Materials**. The Eddy controller stores information about the materials and sources that are available. Each source is numbered and the name of the material is attached, together with other operating details. The Eddy Editor can download this information and edit it and can also store it in **.edm** files. In fact it is possible to maintain many such files. The Load Eddy Materials menu item opens a given Eddy materials file and loads the sources and material names into the Machine Configuration Sources tab. It attempts also to map these names to the existing Essential Macleod active materials database. The appearance of the sources table in a new machine configuration is shown next. The **Source** column shows the Eddy source number together with the name and in the **Material** column the suggested mapping to the current database. All that remains to be done to complete the table is entry of the various tooling factors.



Runsheet

There is a new menu, **Eddy**. The commands in this menu are described below.

Program Parameters asks for information that is for use by the Eddy controller itself.



Program Number will identify the program once it is completed.

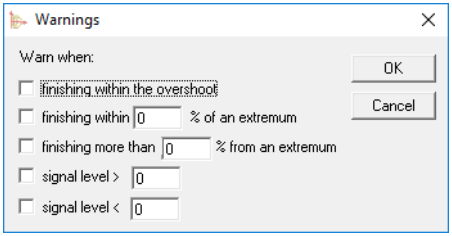
Chip temperature is purely for use by the controller.

Overshoot is the percentage overshoot that must be measured by the controller before it recognizes a peak. This parameter has an immediate influence on the generation of the Runsheet, which will give a warning should any layer be requiring a termination with smaller overshoot.

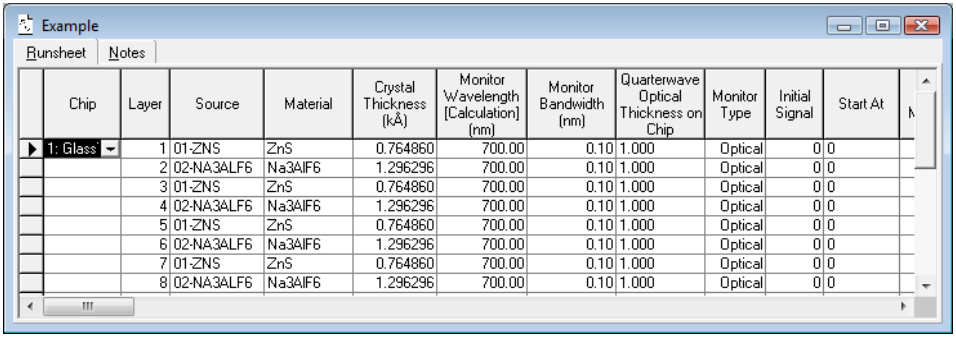
Noise Rejection Level is also an Eddy controller parameter that has an influence on the Runsheet generator. Here the total signal swing must exceed a value that is related to the **Noise Rejection Level**. Again a warning will be given should the necessary condition be infringed.

Note that the presence of these warnings will prevent the exporting of an Eddy program. The warnings must first be cleared.

In the same menu there is also the item **Warnings…** These are warnings identical in type to those in the global Runsheet options but here they are local ones that apply to all layers in the particular active Runsheet only. Some of them are related to the **Program Parameters** just mentioned but here they are more of the nature of desirable targets. They will, of course, trigger warnings just like the others and will prevent export of the program but they can be changed if necessary.

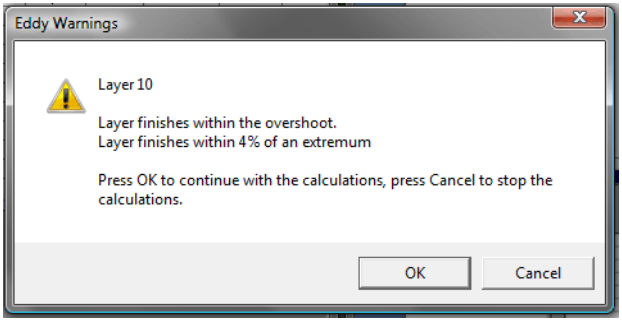


Show Percent Values and **Show Signal Level Values** change from one style of presentation to the other. The percent values correspond to the generic Runsheet while the signal level values correspond to the special form for the Eddy controller. The form of the Runsheet with the signal level values selected is shown in the next figure.



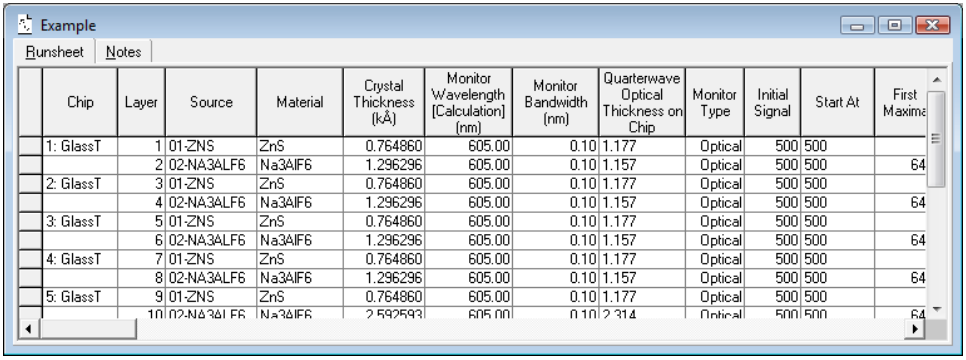
	Chip	Layer	Source	Material	Crystal Thickness (kÅ)	Monitor Wavelength [Calculation] (nm)	Monitor Bandwidth (nm)	Quarterwave Optical Thickness on Chip	Monitor Type	Initial Signal	Start At
▶	1: Glass	1	01-ZNS	ZnS	0.764860	700.00	0.10	1.000	Optical	0	0
		2	02-NA3ALF6	Na3AlF6	1.296296	700.00	0.10	1.000	Optical	0	0
		3	01-ZNS	ZnS	0.764860	700.00	0.10	1.000	Optical	0	0
		4	02-NA3ALF6	Na3AlF6	1.296296	700.00	0.10	1.000	Optical	0	0
		5	01-ZNS	ZnS	0.764860	700.00	0.10	1.000	Optical	0	0
		6	02-NA3ALF6	Na3AlF6	1.296296	700.00	0.10	1.000	Optical	0	0
		7	01-ZNS	ZnS	0.764860	700.00	0.10	1.000	Optical	0	0
		8	02-NA3ALF6	Na3AlF6	1.296296	700.00	0.10	1.000	Optical	0	0

In fact, this design as it stands is not very suitable for monitoring all on one substrate. Warning messages similar to the following are received.



We need to change the monitoring arrangement to use more chips and either to change the tooling factor to move the layer thicknesses away from quarterwaves or to change the wavelength for the same reason. Here we make a small adjustment to the wavelength. With some trial and error we reduce this to 605nm and we deposit only two layers on each chip, the first being of high index.

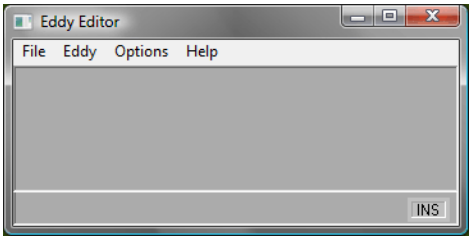
The cut ranges from 6% to 27%(layer 10, the cavity layer) and now the program can be exported.



	Chip	Layer	Source	Material	Crystal Thickness (kÅ)	Monitor Wavelength [Calculation] (nm)	Monitor Bandwidth (nm)	Quarterwave Optical Thickness on Chip	Monitor Type	Initial Signal	Start At	First Maxima
	1: GlassT	1	01-ZNS	ZnS	0.764860	605.00	0.10	1.177	Optical	500	500	
		2	02-NA3ALF6	Na3AlF6	1.296296	605.00	0.10	1.157	Optical	500	500	64
	2: GlassT	3	01-ZNS	ZnS	0.764860	605.00	0.10	1.177	Optical	500	500	
		4	02-NA3ALF6	Na3AlF6	1.296296	605.00	0.10	1.157	Optical	500	500	64
	3: GlassT	5	01-ZNS	ZnS	0.764860	605.00	0.10	1.177	Optical	500	500	
		6	02-NA3ALF6	Na3AlF6	1.296296	605.00	0.10	1.157	Optical	500	500	64
	4: GlassT	7	01-ZNS	ZnS	0.764860	605.00	0.10	1.177	Optical	500	500	
		8	02-NA3ALF6	Na3AlF6	1.296296	605.00	0.10	1.157	Optical	500	500	64
	5: GlassT	9	01-ZNS	ZnS	0.764860	605.00	0.10	1.177	Optical	500	500	
		10	02-NA3ALF6	Na3AlF6	2.592593	605.00	0.10	2.314	Optical	500	500	64

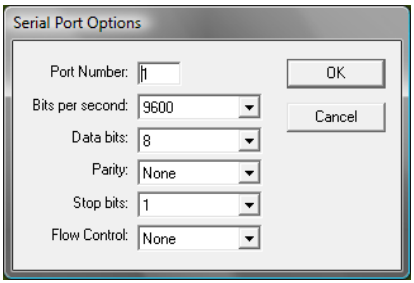
The Eddy LMC-10 Monitorlink Editor

The appearance of the Eddy Editor Application window is shown in the following figure.



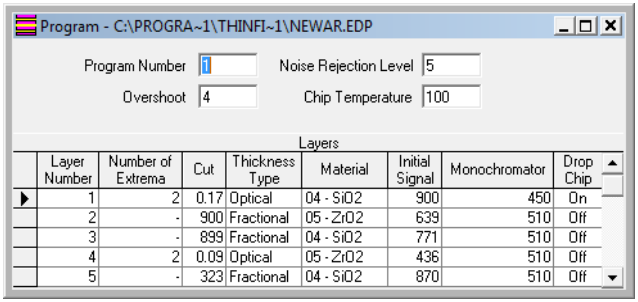
The Menus are described in detail in the Help facility, accessed by selecting **Contents** or **Search for Help on…** in the **Help** menu.

Programs and materials may be stored on the actual controller itself or in a series of files on disk. The File menu concerns those programs and material lists that are actually saved on disk. The Eddy menu concerns those materials and programs that are stored in the controller. The Options menu sets up the details of the serial port for communication with the Eddy controller. The usual settings will be the default ones that are shown in the Serial Port Options dialog that follows.



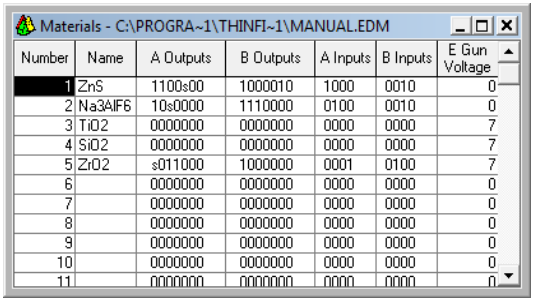
The Password items concern the putting and getting of data to and from the Eddy controller.

The principal menu items from the point of view of the control programs are in the File menu. Here programs may be loaded from the Essential Macleod by selecting **Open Program…** when a selection box for programs exported from the Essential Macleod is presented. Two such programs are shown following. The first is a simple program representing a five-layer antireflection coating. The second is the narrowband filter program that we have been using as an illustration. These programs can be edited in the Eddy Editor in the normal way. Note the toggling of insert and overstrike modes by pressing the insert key as in the Essential Macleod. The Drop Chip column should be considered as referring to the action before the start of deposition of the particular layer. Therefore the entry On means that a fresh chip will be used while Off means that deposition will continue on the existing chip.



Layer Number	Number of Extrema	Cut	Thickness Type	Material	Initial Signal	Monochromator	Drop Chip
1	2	0.17	Optical	04 - SiO2	900	450	On
2	-	900	Fractional	05 - ZrO2	639	510	Off
3	-	899	Fractional	04 - SiO2	771	510	Off
4	2	0.09	Optical	05 - ZrO2	436	510	Off
5	-	323	Fractional	04 - SiO2	870	510	Off

Programs can also be entered manually. The **New** submenu under the **File** menu allows a new set of materials or a new program to be created. The following figure shows a materials list. Each material has a number, from 1 to 99, and a name, the number being the definitive identifier. A and B Outputs and Inputs determine the power, configuration, shutters return signals and so on connected with the particular source. E Gun Voltage is a number from 1 to 10 denoting the voltage in units of 1000V for an electron beam source.



Number	Name	A Outputs	B Outputs	A Inputs	B Inputs	E Gun Voltage
1	ZnS	1100s00	1000010	1000	0010	0
2	Na3AlF6	10s0000	1110000	0100	0010	0
3	TiO2	0000000	0000000	0000	0000	7
4	SiO2	0000000	0000000	0000	0000	7
5	ZrO2	s011000	1000000	0001	0100	7
6		0000000	0000000	0000	0000	0
7		0000000	0000000	0000	0000	0
8		0000000	0000000	0000	0000	0
9		0000000	0000000	0000	0000	0
10		0000000	0000000	0000	0000	0
11		0000000	0000000	0000	0000	0

MONITORLINK for INFICON XTC

Introduction

Monitorlink for the Inficon XTC deposition controller provides facilities for converting an Essential Macleod design into a XTC deposition specification. This deposition specification is uploaded by a separate program into the XTC controller. For specific details about the XTC controller, please refer to the XTC manual.

The mapping of Essential Macleod materials into film parameters for the XTC is defined once by the user. Thereafter, the Essential Macleod automatically converts materials and layer thicknesses into the correct film parameters for the XTC.

Monitorlink provides facilities for managing the film specifications. Films may be added and deleted from the file. Designs may also be edited directly in terms of the XTC film parameters. Complete film definitions may be downloaded from the XTC and saved on a disk.

Using Monitorlink for XTC

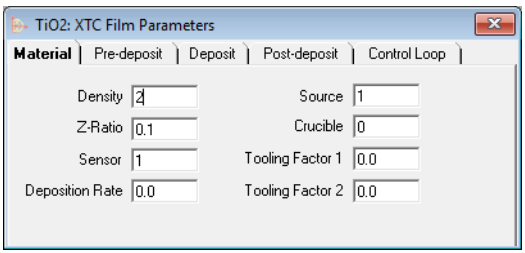
The Monitorlink facilities are provided through the **Tools** menu and through the **File** menu of a design. The Tools menu provides a sub-menu: **XTC**, and this has three options: **Open Film Parameters**, **Open Deposition File** and **New Deposition File**.

Defining a Material Mapping

The material mapping defines the relationship between materials in the Essential Macleod and film parameters in the XTC controller. It is assumed that the only difference between layers of the same material is that the thickness may vary. All other parameters are constant. If the other film parameters are not the same for films of different thicknesses, then either a new material can be created in the Essential Macleod which is then given the different set of parameters, or the film definition can be edited manually. Each materials database has its own mapping from materials to film parameters.

Each material in the Essential Macleod has its own set of film parameters. When **Open Film Parameters** is selected a material chooser is displayed.

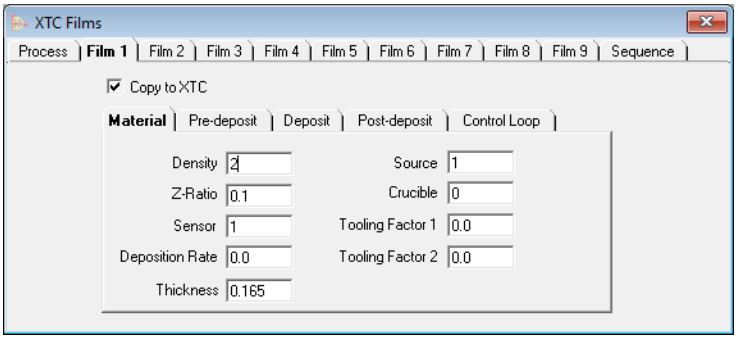
Select the material whose film parameters you wish to define or edit and then click **OK**. The film editor then appears. All of the XTC film parameters may be edited.



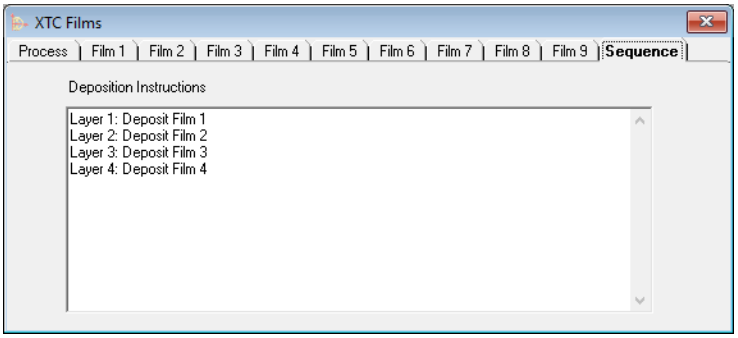
Once all of the XTC film parameters have been edited, the film parameters may be saved by selecting **Save** from the **File** menu. Whenever a design containing layers using this material is converted to an XTC film specification, these parameters will be used in the controller file.

Converting an Essential Macleod Design

In order to convert an Essential Macleod design into an XTC film specification, the film parameters for each of the materials used must have been previously defined. The design is converted by simply selecting **XTC Deposition File** from the **Export** sub-menu of the **File** menu. This will create a new XTC film specification for the design.



When a design contains repeating layers of the same material and thickness such as a quarterwave stack, Monitorlink converts the design into film specifications for each of the unique layer material and thickness combinations, and then writes a deposition sequence instruction for an operator to follow.



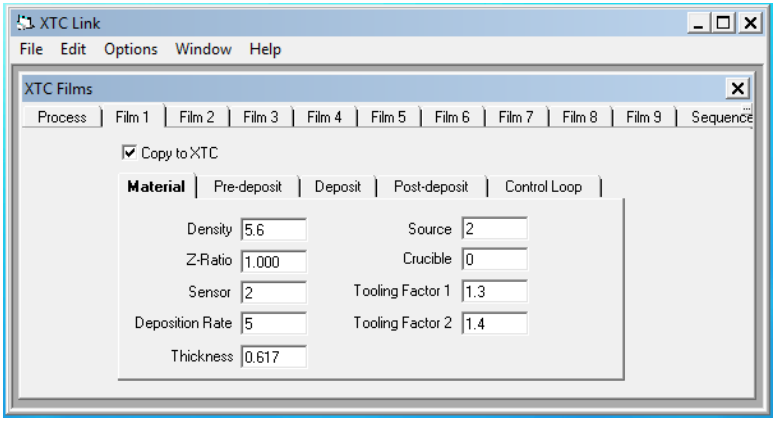
The contents of this file can then be saved ready for uploading to the XTC controller by the XTC communications program – XTC Editor.

Open Deposition File will open an existing deposition file for editing in the Essential Macleod, and **New Deposition File** will create a new deposition file which can be filled with film specifications. In addition to the film specifications and the process definition parameters, the process and film specifications have an extra parameter **Copy to XTC**.

When this parameter is checked, the XTC editor will upload the specification to the XTC controller. If **Copy to XTC** is not checked, then the XTC editor will not upload the film specification or process definition to the XTC controller.

The XTC Editor

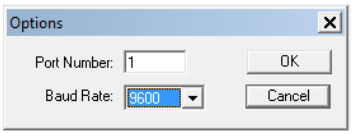
The XTC Editor provides facilities for maintaining and editing complete XTC film specifications. It also provides communications facilities for uploading and downloading film specifications to and from the XTC controller.



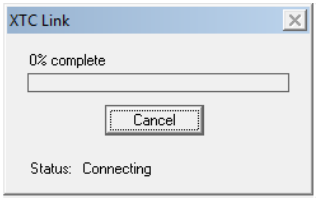
A serial cable (not provided) is required to allow the XTC editor to communicate with the XTC controller. The XTC manual contains details on the specification of this cable.

The XTC Editor can open film specifications saved in the Essential Macleod. These specifications can then be uploaded to the XTC.

Before a film specification can be uploaded, or downloaded, the serial link information must be specified. This is performed by selecting **Options**. The **Port Number** is the serial port number used on the computer. The **Baud Rate** must be the same as defined on the XTC.



Once the Options have been set up, the XTC Editor is ready to communicate with the XTC controller. To upload a film specification to the XTC controller, select **Send to XTC** from the **File** menu.



Progress in sending the film specifications to the XTC is shown. When completed, the progress form disappears. If there are any problems in sending the data, an error message will be displayed. Often the problem can be resolved by checking the serial cable connecting the computer to the XTC and resetting the XTC by turning it off and then on again. Occasionally, it may be necessary to restart the XTC editor to clear the problem.

Films may be downloaded from the XTC by selecting **Get from XTC** from the File menu. A new film specification window will be created containing the downloaded data. This can be saved to disk in the usual manner.

MONITORLINK for APPLIED VISION PLASMACOAT

Introduction

Monitorlink for Applied Vision Ltd's PlasmaCoat coating system provides facilities for converting an Essential Macleod design into a PlasmaCoat production specification. This production specification is automatically placed, by the Essential Macleod, into the Players.dat file used by the PlasmaCoat system.

The mapping of Essential Macleod materials into control parameters for the PlasmaCoat system is defined once by the user. Thereafter, the Essential Macleod automatically converts materials and layer thicknesses into the correct control parameters for the PlasmaCoat system.

A pre-deposition phase may also be specified. The pre-deposition phase may be used, for example, to perform substrate cleaning or deposition of a thin adhesion layer. The predeposition phase is always inserted in the production specification before the design's layers are specified.

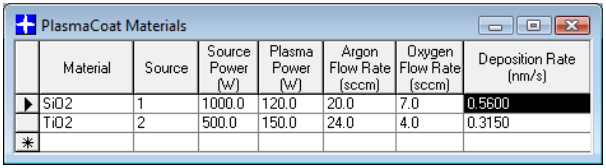
Monitorlink provides facilities for managing the contents of the Players.dat file. Production specifications may be added and deleted from the file. Designs may also be edited directly in terms of the PlasmaCoat control parameters.

Using Monitorlink for PlasmaCoat

The Monitorlink facilities are provided through the **Tools** menu and through the **File** menu of a design. The Tools menu provides a sub-menu: **PlasmaCoat**, and this has three options: **Open Materials**, **Open Predeposition Phase** and **Open Design File**.

Defining a Material Mapping

Open Materials displays a window that defines the mapping between the Essential Macleod materials and the PlasmaCoat control parameters. Each materials database has its own mapping from materials to control parameters.

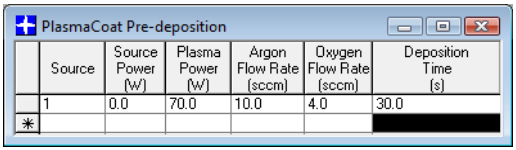


	Material	Source	Source Power (W)	Plasma Power (W)	Argon Flow Rate (sccm)	Oxygen Flow Rate (sccm)	Deposition Rate (nm/s)
▶	SiO2	1	1000.0	120.0	20.0	7.0	0.5600
	TiO2	2	500.0	150.0	24.0	4.0	0.3150
✳							

Each line in the Materials display defines a mapping from a single material to the PlasmaCoat control parameters. For a description of the PlasmaCoat parameters, please refer to the PlasmaCoat documents.

Defining a Predeposition Phase

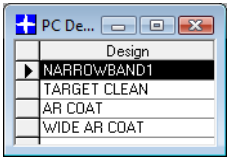
Open Predeposition Phase displays the predeposition phase that will be applied to all designs that are converted from the Essential Macleod format. The predeposition phase is defined as a sequence of PlasmaCoat control parameters that are executed starting with the top row and then proceeding down the list. A predeposition phase need not be defined, in which case, only the design's layers will be present in the resulting Players.dat file.



The figure above shows a predeposition phase consisting of thirty seconds of substrate cleaning.

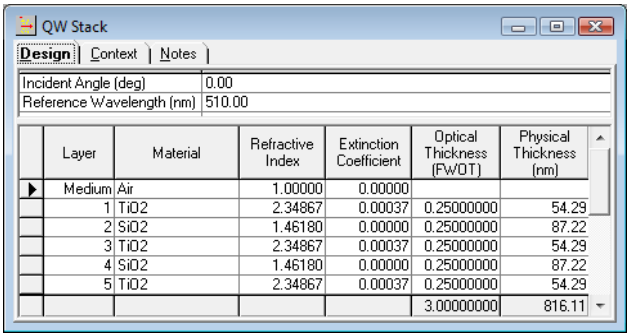
Converting an Essential Macleod Design

In order to convert an Essential Macleod design into a PlasmaCoat specification, the PlasmaCoat players.dat file must first be loaded into the Essential Macleod. This is achieved through the Open Design File menu option. After the user has selected the Players.dat file to be loaded, a list of the designs contained in the Players.dat file is displayed

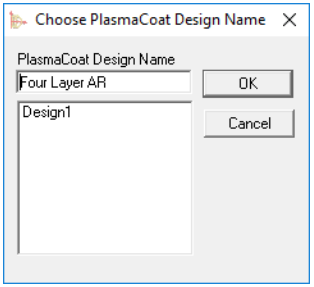


With the design file loaded, an Essential Macleod design may be added to the PlasmaCoat design list. Also, designs may be edited, deleted and renamed.

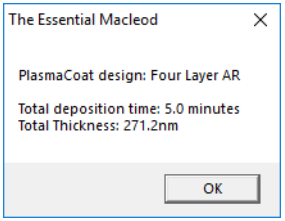
As an example, a small quarterwave stack will be added to the design file. The design is shown below



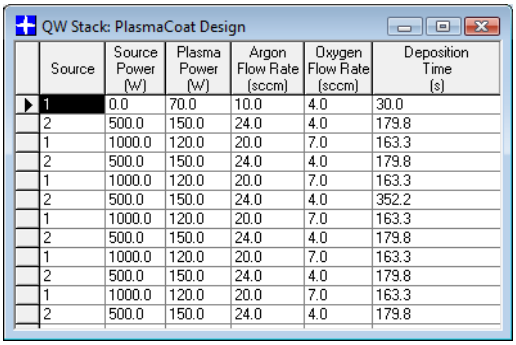
To convert the design, select **Export** in the **File** menu and then select **PlasmaCoat Design**. You will then be asked to enter the name of the design to be used in the PlasmaCoat file. By default, this name will be the same as the name of the Essential Macleod design.



After clicking **OK**, the design will be converted and loaded into the PlasmaCoat designs window. At this stage the PlasmaCoat design has not been saved to disk. You will be informed of the total thickness of the design and the deposition time including any predeposition phase.



The PlasmaCoat specification of the design can now be viewed by double-clicking on the design name in the PlasmaCoat Designs window.



	Source	Source Power (W)	Plasma Power (W)	Argon Flow Rate (sccm)	Oxygen Flow Rate (sccm)	Deposition Time (s)
▶	1	0.0	70.0	10.0	4.0	30.0
	2	500.0	150.0	24.0	4.0	179.8
	1	1000.0	120.0	20.0	7.0	163.3
	2	500.0	150.0	24.0	4.0	179.8
	1	1000.0	120.0	20.0	7.0	163.3
	2	500.0	150.0	24.0	4.0	352.2
	1	1000.0	120.0	20.0	7.0	163.3
	2	500.0	150.0	24.0	4.0	179.8
	1	1000.0	120.0	20.0	7.0	163.3
	2	500.0	150.0	24.0	4.0	179.8
	1	1000.0	120.0	20.0	7.0	163.3
	2	500.0	150.0	24.0	4.0	179.8

This window shows the quarterwave stack converted to a PlasmaCoat specification The predeposition phase defined above has also been added to the PlasmaCoat specification.

The set of PlasmaCoat designs can be saved to disk by the **Save** command, or the **Save As** command if a new file name is desired, in the **File** menu.

MONITORLINK for LEYCOM IV with OMS3000

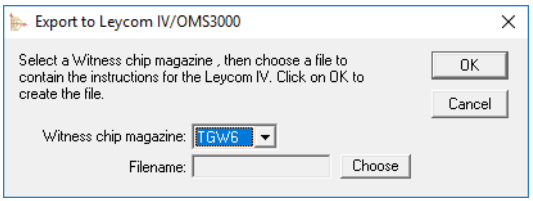
Introduction

The Monitorlink for Leycom IV with OMS3000 provides the ability to create a process data file for import into the remote control software for the Leycom IV.

Modifications to Runsheet

This Monitorlink converts data held in Runsheet and its associated Machine Configuration into a process data file suitable for import into the remote control software for the Leycom IV.

To start the export, select the **Leybold IV/OMS3000** command in the **Export** menu, which is a sub-menu of the **File** menu. The export parameters form will be displayed.



The form must be completed with the extra information required to complete the export process. Three types of witness chip are supported: TGW6, TGW50 and TGW100. The TGW6 has six chips that may be reused during the deposition process. The TGW50 has 50 chips, but the chips may not be reused during the deposition process. The TGW100 has 100 chips, but the chips may not be reused during the deposition process. The Filename is the name of the file that will contain the process data. Click **Choose** to specify the filename.

Clicking the **OK** button will cause the Runsheet to be checked for errors. If there are no errors, the process data file will be written. Clicking the **Cancel** button will abort the export process.

The process data file is built as follows: The step number always starts at 1. The layer set name used in the process data file will be the name of the source in the machine configuration used by the Runsheet. The optical thickness is the value given in the Optical Thickness on Monitor Chip column of the Runsheet. This is the optical thickness at the monitoring center wavelength. The refractive index at the monitoring center wavelength is the refractive index to be used by the optical monitor. The witness chip column contains the chip number to be used when the TGW6 magazine has been specified. When the TGW50 or TGW100 magazines have been specified, the witness chip column contains a 1 to indicate that a new chip is required and a 0 where the chip is not changed.

MONITORLINK for INFICON IC/5

Introduction

Monitorlink for the Inficon IC/5 deposition controller provides facilities for converting an Essential Macleod design into an IC/5 process specification. This process specification is uploaded by a separate program into the IC/5 controller. For specific details about the IC/5 controller, please refer to the IC/5 manual.

The software assumes that, normally, all layer parameters in the IC/5 apart from thickness are the same for each layer of the same material in the Essential Macleod. Thus, when a design is exported to the IC/5, the Essential Macleod will look up layer parameters according to the material used for each layer and add in the thickness of each layer. Conversion to kiloAngstrom units is performed automatically. The mapping of Essential Macleod materials into layer parameters for the IC/5 is defined once by the user. Each materials database contains its own set of layer parameters. If you have several IC/5 controllers that use different layer parameters for the same material, then you should set up a separate materials database for each IC/5. Using the correct materials database before exporting a design will ensure that the correct layer parameters are used.

If you already have layer parameters setup in the IC/5 controller, you can download them using the IC/5 and save the process data to disk. In the Essential Macleod, you can open the process data file and copy a layer parameter set. To associate the layer parameter set with a particular material, open the IC/5 material parameters for the material and then use the paste command in the edit menu. All the parameters apart from the layer thickness will be copied into the material information. See below for more information.

Monitorlink provides facilities for managing the film specifications. Films may be added and deleted from the file. Designs may also be edited directly in terms of the IC/5 film parameters. Complete process definitions may be downloaded from the IC/5 and saved on a disk.

Using Monitorlink for IC/5

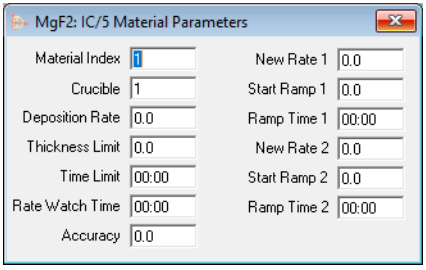
The Monitorlink facilities are provided through the **Tools** menu and through the **File** menu of a design. The Tools menu provides a sub-menu: **IC/5**, and this has three options: **Open Material Parameters**, **Open Process File** and **New Process File**.

Defining a Material Mapping

The material mapping defines the relationship between materials in the Essential Macleod and layer parameters in the IC/5 controller. It is assumed that the only difference between layers of the same material is that the thickness may vary. All other parameters are constant. If the other layer parameters are not the same for layers of different thicknesses, then either a new material can be created in the Essential Macleod which is then given the different set of parameters, or the layer definition can be manually edited. Each materials database has its own mapping from Essential Macleod materials to IC/5 layer parameters.

To modify the layer parameters for a particular material, select **Open Material Parameters** from the **IC/5** sub-menu of the **Tools** menu. A material chooser is then displayed.

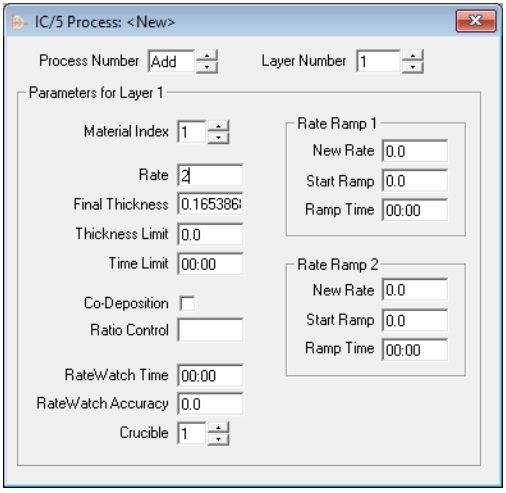
Select the material whose layer parameters you wish to define or edit and then click **OK**. The layer editor then appears. All of the IC/5 layer parameters (apart from thickness) may be edited.



Once all of the IC/5 layer parameters have been edited, the layer parameters may be saved by selecting **Save** from the **File** menu. Whenever a design containing layers using this material is converted to an IC/5 layer specification, these parameters will be used in the process file.

Converting an Essential Macleod Design

In order to convert an Essential Macleod design into an IC/5 film specification, the layer parameters for each of the materials used must have been previously defined. The design is converted by simply selecting **IC/5 Deposition File** from the **Export** sub-menu of the **File** menu. This will create a new IC/5 process specification for the design.



The contents of this file can then be saved ready for uploading to the IC/5 controller by the IC/5 communications program – IC/5 Editor.

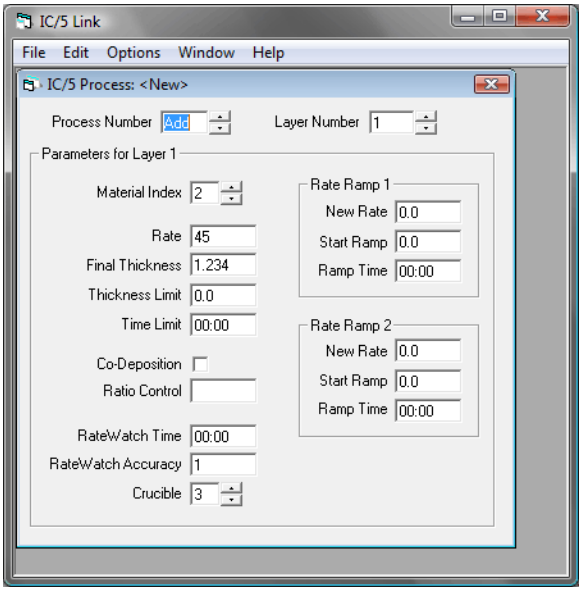
Open Process File will open an existing process file for editing in the Essential Macleod, and **New Process File** will create a new process file which can be filled with layer specifications.

The IC/5 Editor

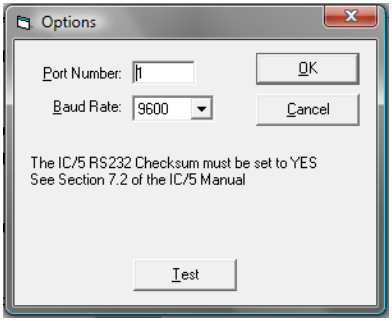
The IC/5 Editor provides facilities for maintaining and editing complete IC/5 process specifications. It also provides communications facilities for uploading and downloading process specifications to and from the IC/5 controller.

A serial cable (not provided) is required to allow the IC/5 editor to communicate with the IC/5 controller. The IC/5 manual provides the specification of this cable.

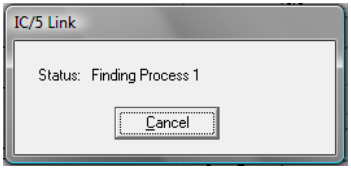
The IC/5 Editor can open process specifications saved in the Essential Macleod. These specifications can then be uploaded to the IC/5.



Before a layer specification can be uploaded, or downloaded, the serial link information must be specified. This is performed by selecting **Options**. The **Port Number** is the serial port number used on the computer. The **Baud Rate** must be the same as defined on the IC/5.



Once the Options have been set up, the IC/5 Editor is ready to communicate with the IC/5 controller. To upload a layer specification to the IC/5 controller, select **Send to IC/5** from the **File** menu.



Progress in sending the process specification to the IC/5 is shown. When completed, the progress display disappears. If there are any problems in sending the data, an error message will be displayed. Often the problem can be resolved by checking the serial cable connecting the computer to the IC/5 and resetting the IC/5 by turning it off and then on again. Occasionally, it may be necessary to restart the IC/5 editor to clear the problem.

Process specifications may be downloaded from the IC/5 by selecting **Get all processes from IC/5** from the File menu. A new Process specification window will be created for each downloaded process. These can be saved to disk in the usual manner.

MONITORLINK for Sycon STC

Introduction

Monitorlink for the Sycon STC deposition controller provides facilities for converting an Essential Macleod design into a STC deposition specification. This deposition specification is uploaded by a separate program into the STC controller. For specific details about the STC controller, please refer to the STC manual.

The mapping of Essential Macleod materials into film parameters for the STC is defined once by the user. Thereafter, the Essential Macleod automatically converts materials and layer thicknesses into the correct film parameters for the STC.

Monitorlink provides facilities for managing the film specifications. Films may be added and deleted from the file. Designs may also be edited directly in terms of the STC film parameters. Complete film definitions may be downloaded from the STC and saved on a disk.

Using Monitorlink for STC

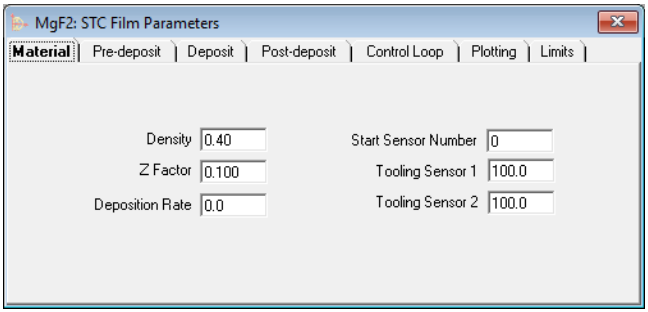
The Monitorlink facilities are provided through the **Tools** menu and through the **File** menu of a design. The Tools menu provides a sub-menu: **STC**, and this has three options: **Open Film Parameters**, **Open Deposition File** and **New Deposition File**.

Defining a Material Mapping

The material mapping defines the relationship between materials in the Essential Macleod and film parameters in the STC controller. It is assumed that the only difference between layers of the same material is that the thickness may vary. All other parameters are constant. If the other film parameters are not the same for films of different thicknesses, then either a new material can be created in the Essential Macleod which is then given the different set of parameters, or the film definition can be edited manually. Each materials database has its own mapping from materials to film parameters.

Each material in the Essential Macleod has its own set of film parameters. When **Open Film Parameters** is selected a material chooser is displayed.

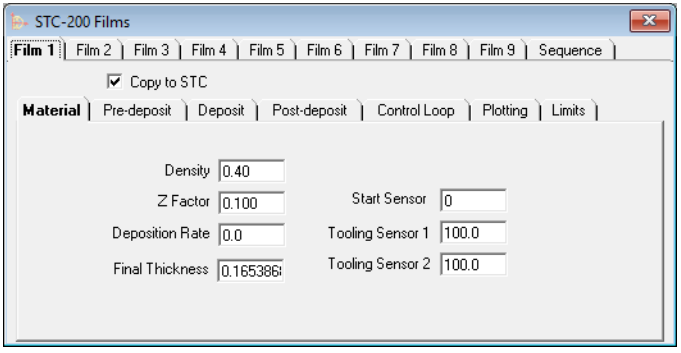
Select the material whose film parameters you wish to define or edit and then click **OK**. The film editor then appears. All of the STC film parameters may be edited.



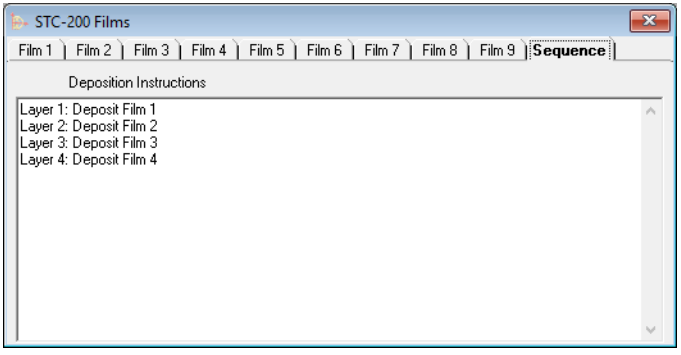
Once all of the STC film parameters have been edited, the film parameters may be saved by selecting **Save** from the **File** menu. Whenever a design containing layers using this material is converted to an STC film specification, these parameters will be used in the controller file.

Converting an Essential Macleod Design

In order to convert an Essential Macleod design into an STC film specification, the film parameters for each of the materials used must have been previously defined. The design is converted by simply selecting **STC Deposition File** from the **Export** sub-menu of the **File** menu. This will create a new STC film specification for the design.



When a design contains repeating layers of the same material and thickness such as a quarterwave stack, Monitorlink converts the design into film specifications for each of the unique layer material and thickness combinations, and then writes a deposition sequence instruction for an operator to follow.



The contents of this file can then be saved ready for uploading to the STC controller by the STC communications program – STC Editor.

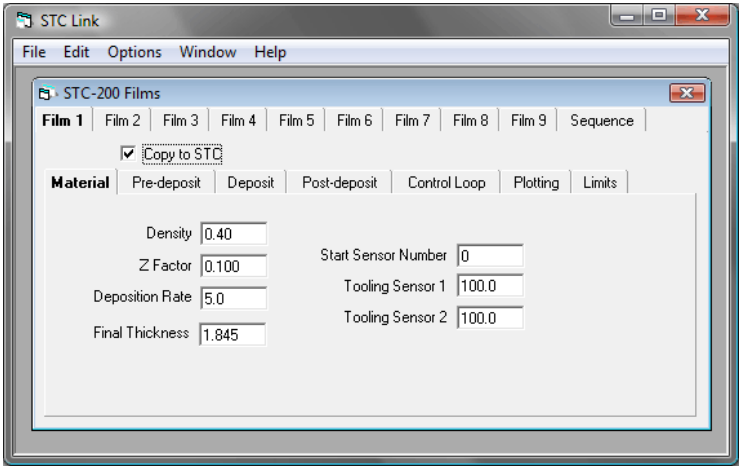
Open Deposition File will open an existing deposition file for editing in the Essential Macleod, and **New Deposition File** will create a new deposition file which can be filled with film specifications. In addition to the film specifications, there is an extra parameter **Copy to STC**. When this parameter is checked, the STC editor will upload the specification to the STC controller. If **Copy to STC** is not checked, then the STC editor will not upload the film specification to the STC controller.

The STC Editor

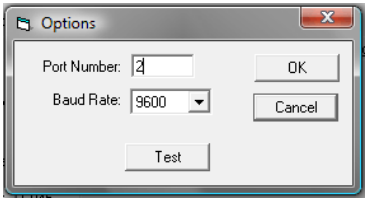
The STC Editor provides facilities for maintaining and editing complete STC film specifications. It also provides communications facilities for uploading and downloading film specifications to and from the STC controller.

A serial cable (not provided) is required to allow the STC editor to communicate with the STC controller. The STC manual contains details on the specification of this cable.

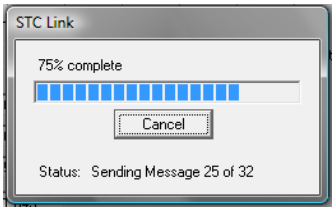
The STC Editor can open film specifications saved in the Essential Macleod. These specifications can then be uploaded to the STC.



Before a film specification can be uploaded, or downloaded, the serial link information must be specified. This is performed by selecting **Options**. The **Port Number** is the serial port number used on the computer. The **Baud Rate** must be the same as defined on the STC.



Once the Options have been set up, the STC Editor is ready to communicate with the STC controller. To upload a film specification to the STC controller, select **Send to STC** from the **File** menu.



Progress in sending the film specifications to the STC is shown. When completed, the progress form disappears. If there are any problems in sending the data, an error message will be displayed. Often the problem can be resolved by checking the serial cable connecting the computer to the STC and resetting the STC by turning it off and then on again. Occasionally, it may be necessary to restart the STC editor to clear the problem.

Films may be downloaded from the STC by selecting **Get from STC** from the File menu. A new film specification window will be created containing the downloaded data. This can be saved to disk in the usual manner

MONITORLINK for SC Technology 820

Introduction

Monitorlink for the SC Technology 820 optical monitor provides adds monitoring data to be used by the SC Technology 820 to the Runsheet file. For specific details about the 820 optical monitor, please refer to the SC Technology 820 manual.

Using Monitorlink for SC Technology 820

The data that are used by the SC Technology 820 are held in the Runsheet file.

The wavelengths that are to be used are specified by the Machine Configuration used by Runsheet. In the Machine Configuration Editor, you can specify the wavelength range on the **Wideband** tab.

The Runsheet menu in the Runsheet editor contains commands for plotting the spectral data. These commands are discussed in the Runsheet chapter of this manual.

MONITORLINK for LEYBOLD LMR & LDD Compatible Systems

Introduction

Some Leybold coating machines (including the SYRUS*pro* and Helios) support communication of monitoring information and material dispersion data via two Leybold defined file formats: Leybold Monitoring Report and Leybold Dispersion Data. The Essential Macleod can import and export both of these Leybold formats.

Materials

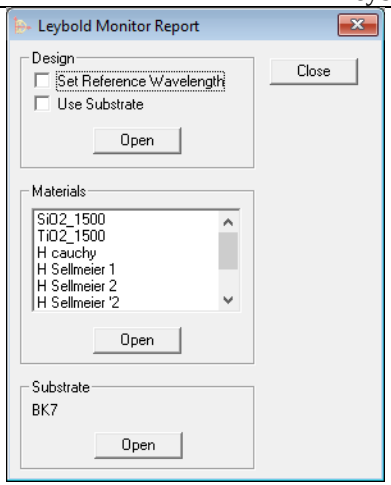
Material dispersion data are communicated in the Leybold Dispersion Data file. This file normally has a .ldd extension. To create an ldd file from an existing material, open the material. From the File menu, select Export and then Leybold LDD… A file chooser will be displayed. Enter the name of the ldd file and click Save. This will write the material data into the file in the ldd format.

The data in an ldd file can also be imported as a new material. To open an ldd file, select Open from the File menu. A file chooser will be displayed. Change the Files of type to All files (*.*). Select the ldd file and click Open. The ldd material data will appear in a new material window.

Runsheet

Runsheet data are communicated in the Leybold Monitoring Report file. This file normally has a .lmr extension. To create an lmr file from an existing runsheet, open the runsheet. From the File menu, select Export and then Leybold LMR… A file chooser will be displayed. Enter the name of the lmr file and click Save. This will write the runsheet data into the file in the lmr format. Note: In use, the XML schema file (.xsd extension) that is used by, and supplied with, the Leybold software, should be in the same folder as the LMR file.

The data in an lmr file can also be imported into the Essential Macleod. The lmr file contains material data and the design. To open an lmr file, select Open from the File menu. A file chooser will be displayed. Change the Files of type to All files (*.*). Select the lmr file and click Open. The window below will appear.



The buttons on this window are used to open the various elements of the lmr file. To open a material definition in the list, select the material by clicking on it and then click Open Material to display the data in a new material window.

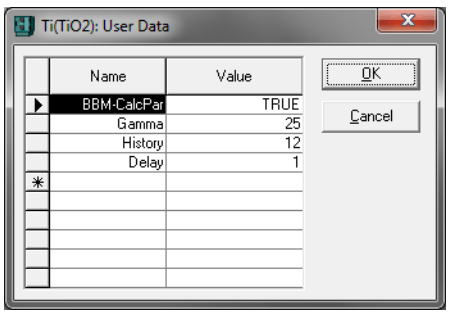
MONITORLINK for Laser Zentrum Hannover Broadband Optical Monitor

Introduction

Data can be loaded into the Laser Zentrum optical monitor from a Spektrum formatted file. As well as design information, this format can include optical monitor parameters such as Rate, Gamma, History, and Delay for each material and up to five wavelength ranges with weights where the optical monitor is to collect data. All this information can be stored by the Essential Macleod and exported from a Runsheet. A Spektrum file can also be exported from the Design window, but in this case the Runsheet-related information cannot be included.

Machine Configuration

The Machine Configuration is used to store the material-related optical monitor parameters: Rate, BBM-CalcPar, Gamma, History and Delay. The Deposition Rate data is taken from the Machine Configuration's **Deposition Rate** column in the **Sources** tab. The other information is entered via a separate dialog. To enter this information, select a source by clicking in the gray box at the left end of the appropriate Source row. Then from the **Edit** menu select **Edit User Data…** The Edit User Data window will appear.



For each parameter, enter its name in the **Name** column and the value to be associated with the parameter in the **Value** column. During export, these values will be written to the Spektrum file along with the material data. Note that the names must be exactly as written here. Any other name/value pairs will not be exported.

The full bandwidth of the optical monitor must be specified on the **Wideband** tab of the Machine Configuration. **Wideband Available** must also be checked. The **Wavelength Interval** is not exported but is used during wideband calculations in Runsheet.

Runsheet

The optical monitor can measure spectral data from up to five wavelength regions per layer. These wavelength regions can be defined in Runsheet using the Wavelength Range columns. Each of the five wavelength range column sets can be individually displayed using the **Display Setup** command in the **File** menu. There are three columns

in each column set: **Wavelength Start**, **Wavelength End** and **Weight**. For more information about these parameters, please consult the optical monitor's manual. Values entered in these columns will be exported to the Spektrum file. Additionally, the Wideband plotting commands in the **Runsheet** menu will show the locations of the wavelength ranges on the plots. Wavelengths within the specified ranges will be shown in the usual colors. Wavelengths outside all ranges will be shown using a faded color with boundary markers at each wavelength edge.

To export the Runsheet, select **Spektrum Design…** from the **Export** menu located in the **File** menu and provide the requested filename.

THE ESSENTIAL MACLEOD LICENSE SYSTEM

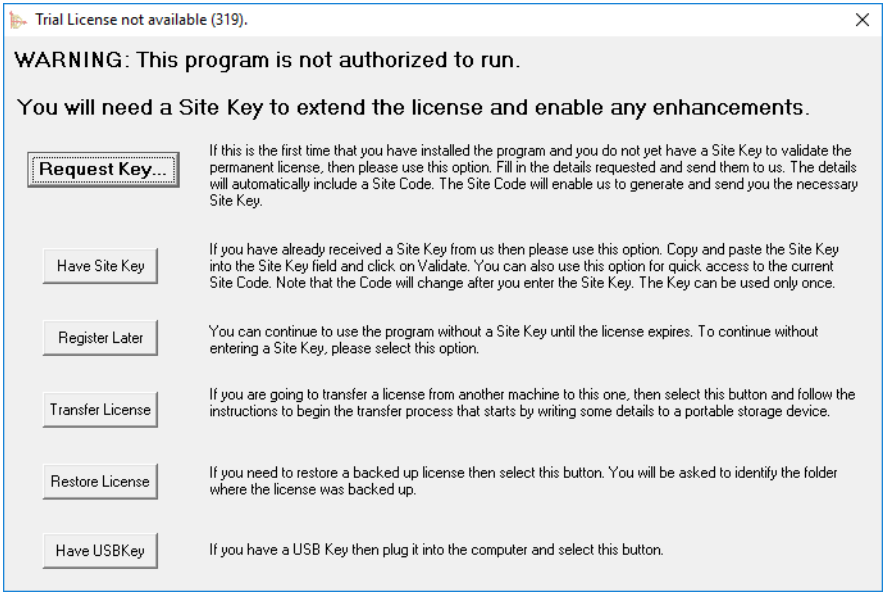
Introduction

The Essential Macleod has a built-in licensing system. When the Essential Macleod is fully licensed, it operates invisibly. After initial installation of the Essential Macleod, the software is licensed for a 15-day period. This allows you to use the software as soon as you have installed it, and allows time for you to obtain the full license. When the software is not fully licensed, you will be reminded, each time you start the Essential Macleod, of the number of days left on the initial license. There are two types of license available: a Transferable License or a Fixed License. A transferable license can be moved from one computer to another (by following the instructions below). A fixed license cannot be transferred from one computer to another, but you can make a backup copy of the license. A fixed license is only available for certain computers. Availability can only be determined after the key request has been made.

Obtaining a Full License

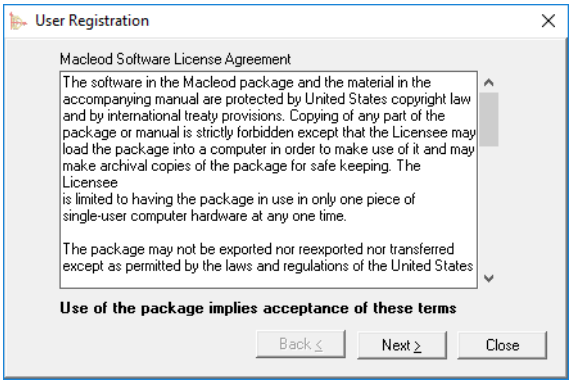
To obtain a Full License, you must register the Essential Macleod. Thin Film Center will then supply you with a key that must be entered into the Essential Macleod. Once the key has been successfully entered, the program will be fully licensed. Telephone, fax or e-mail can be used for transferring the information between you and Thin Film Center.

To register the Essential Macleod either click **Request Key…** on the Limited License message that appears when you start the Essential Macleod,

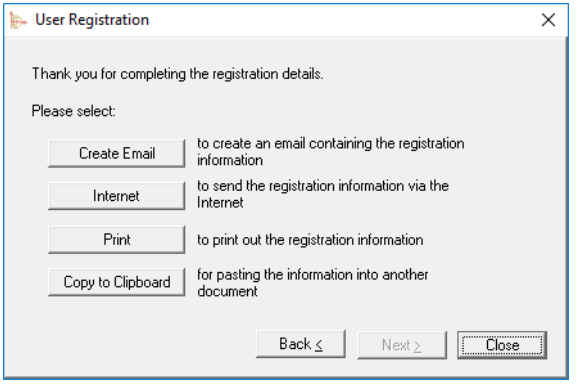


or select **Register** from the **Options** menu of the Essential Macleod.

The registration window will appear. The registration window contains a series of pages to be read and completed. The first page contains the license agreement. When you register the software, you accept the terms of the license agreement.



Click **Next** to advance to the next page. On this page and the next three pages you will be asked to enter your user information and any comments. You will also be shown information that will be included with the registration data. The final page presents you with several options for sending the data to Thin Film Center.

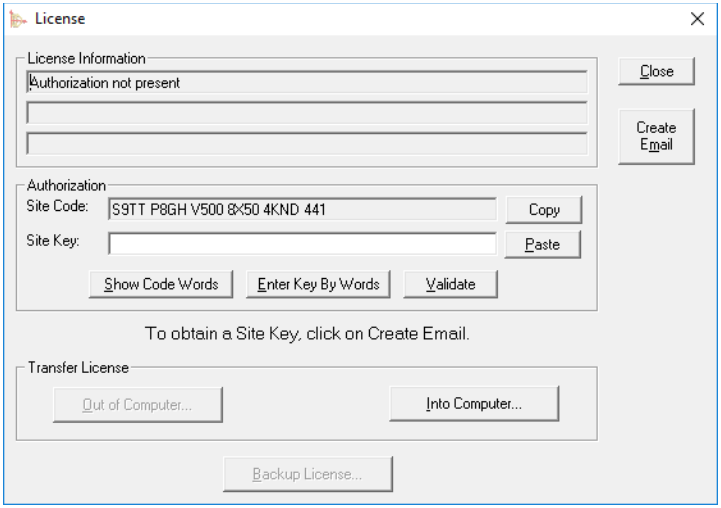


Depending upon the setup of your computer, some of these options may not be available.

You can click the **Internet** button to send the data to Thin Film Center. **Print** will print out the data on your printer together with the fax number. **Copy to Clipboard** will put the registration data onto the clipboard so that you can paste it into another document. The best method for registration is send the data via the Internet, either by using the Internet button or by copying the data into a message in your e-mail program.

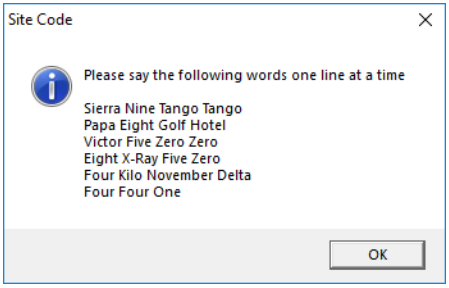
When you have sent the registration to Thin Film Center, you will receive a Site Key. This is a set of letters and digits that must be entered into the Essential Macleod. To enter

the key, either select **Have Site Key** from the Limited License message that appears when you start the Essential Macleod or select **License** from the **Options** menu. The license form will appear.



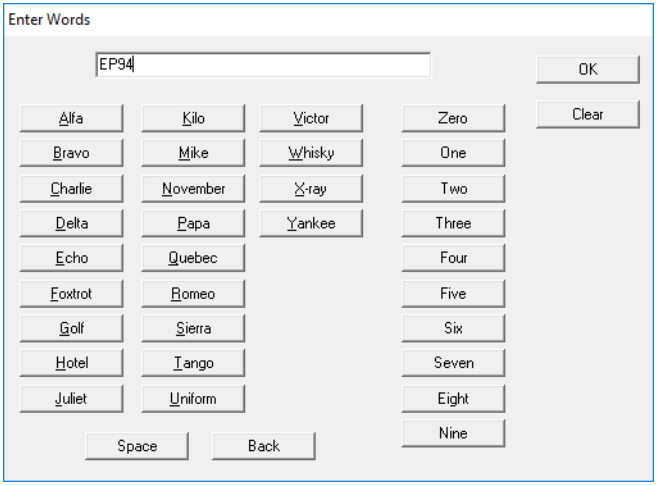
The form gives information about the status of your license. Paste or enter the Site Key into the Site Key field on this form and then click **Validate**. If you use the **Paste** button, the key will automatically be validated after it has been pasted. You will then get a message stating that the Site Key was accepted. Click **OK** in this message and then click **Close** in the License window. You can now use the Essential Macleod.

If you urgently need a key, you can contact Thin Film Center by telephone. As it can be difficult to correctly hear letters spoken over the telephone, we recommend the use of the international phonetic alphabet. When you are asked to read out the Site Code, please click **Show Code Words**. This will display a window that has the Site Code written out as words.



Please read these words, one line at a time, to the Thin Film Center representative. If you are not familiar with the phonetic alphabet, you can click Enter Key by Words. This

will display a window containing buttons labeled with the words that you will hear when the key is being read to you.



As you hear each word, click the button labeled with the word. If you make a mistake, you can click the **Back** button to erase the last entered character. When you have completed entering the Key, click **OK**. The window will close and the Site Key field will have the key entered into it. Click **Validate**. You will then get a message stating that the Site Key was accepted. Click **OK** in this message and then click **Close** in the License window.

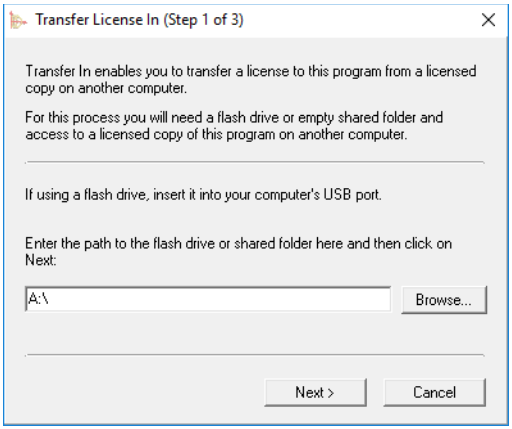
A Site Key can only be used once. After you have entered the Site Key, the Site Code will change and the key will not work.

Transferring the License to another Computer

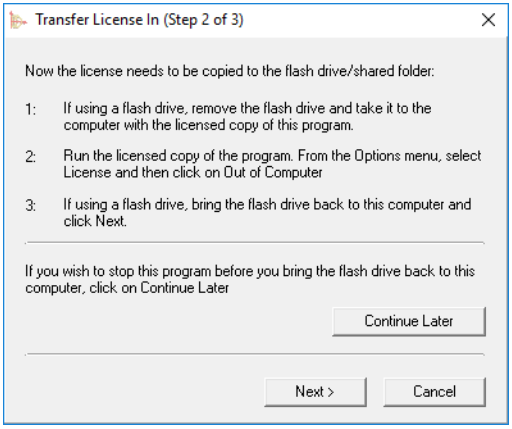
An Essential Macleod transferable license may be transferred from one computer to another. The transfer process can be performed using a folder that is accessible to both computers (if the computers are networked), or it can be performed using a removable storage device.

The license transfer process starts at the computer that is to receive the license. With the Essential Macleod running and no windows open on the Essential Macleod background window, select **License** from the **Options** menu. Then select **Start Transfer** on the License form that appears. The Start Transfer form will appear.

To start the license transfer, either select **Transfer License** from the Limited License message that appears when you start the Essential Macleod or select **License** from the **Options** menu, and then click the **Into Computer** button. The Transfer License In form will appear.

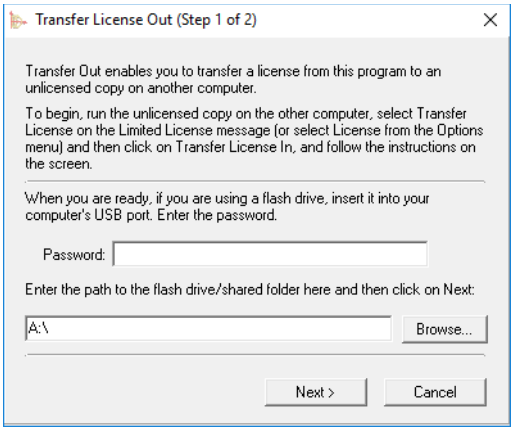


Enter the folder that is to be used for the license transfer and then select **Next**. If successful, the following window will appear



You can either leave the Essential Macleod running while you get the license from the other computer, or you can click **Continue Later** to suspend the Transfer In process. This allows you to stop the Essential Macleod. You can continue the Transfer In process at another time.

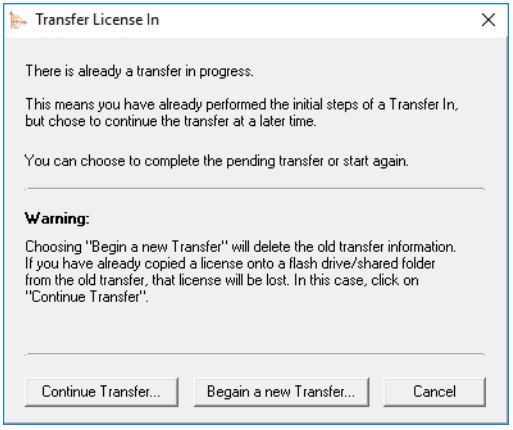
Now move to the computer from which the license will be taken. If a removable storage device was used for the transfer process, insert the device into the computer. Run the Essential Macleod. With no windows open on the Essential Macleod desktop, select **License** from the **Options** Menu. Select **Out of Computer** on the license form.



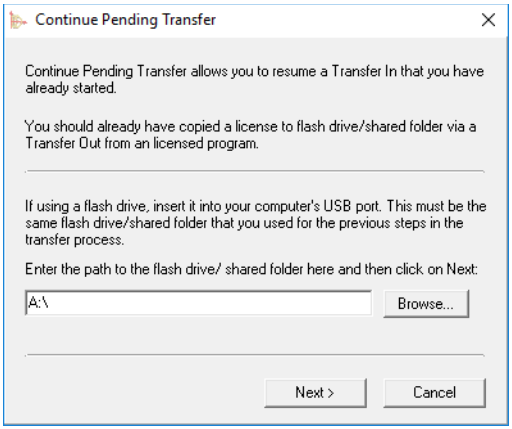
Transferring out a license from the Essential Macleod is password protected (On first installation of the Essential Macleod, the password is blank and so you can leave the password field blank). Change the transfer folder if necessary and then click **Next**. The license will now be moved to the transfer folder. It cannot be moved back from the transfer folder to the computer, it can only be moved to the unlicensed computer.

Now move back to the computer that is to receive the license. If a removable storage device was used for the transfer process, insert the device into the computer. If you left the Essential Macleod running at Transfer License In (Step 2 of 3), click **Next** to transfer the license into the computer.

If you stopped the Essential Macleod during the transfer in process by clicking the **Continue Later** button, start the Essential Macleod and click the **Transfer License** button on the Limited License message. The Transfer License In form will be displayed.



Click the **Continue Transfer** button.



Enter the transfer folder and select **Next**. The computer should now have the Essential Macleod license.

If you have started a transfer but decide not to complete it, you can click **Begin a new Transfer**, This will discard the current transfer information. If you have already transferred a license out of a computer and you select this option, and accept the warnings, you will lose the license – it cannot be recovered.

Changing the Password

The password for transferring out a license may be altered through the Change Password form. After all windows in the Essential Macleod have been closed, and only the Essential Macleod background window is visible, select **Change Password** from the Options menu. To change the password, you need to enter the current password and then the new password twice. Select **OK** to change the password or select **Cancel** to stop the password from changing.

On first installation, the password is blank.

Backing and Restoring a Fixed License

A Fixed license can be backed up to a separate location and restored to the computer in the event that the license data is lost.

With the Essential Macleod running and no windows open on the Essential Macleod background window, select **License** from the **Options** menu. Then click **Backup License** (**Backup License** will only be available if you have a fixed license). A folder chooser will appear. Select the folder where you want the license to be saved. This can be a location on your computer, removable storage or an accessible network location. Click **OK**. A message will state that the license has been successfully backed up.

If the license is not present, you will see the Limited License message when you start the Essential Macleod. Click the **Restore License** button. A folder chooser will appear.

Select the location of the backup copy of the license and click **OK**. When the license is successfully restored, the Essential Macleod will start.

Warning

This warning only applies to transferable licenses.

The licensing process maintains four files in a license folder. The location of the license folder depends upon when the Essential Macleod was first installed and how the computer is setup. The location of the files is given at the end of the installation. These files are named **essental.41s**, **essental.ent**, **essental.key** and **essental.rst**. These files should not be touched. If they are deleted, then the license will be lost. If this happens, please contact Thin Film Center for assistance.

Some disk defragmenter programs, particularly Norton Speed Disk (version 4 and greater) will move system files as well as ordinary files. Before using your defragmenter, please configure it so that it does not move the essental.ent, essental.key, essental.rst and essental.41s files in the license folder. Consult your de-fragmenter software manual for more information about preventing files from being re-located. Please contact Thin Film Center if you have any questions. (Telephone: +1 520 322 6171, e-mail: info@thinfilmcenter.com

INDEX