RefDex v1.3 User Manual

Contents

1 Introduction

This document is inteded as a reference guide to the functionality of the RefDex modelling software. This software has two principle uses or modes of operation. Firstly it can simulate the outcome of an optial experiment (e.g. Reflection and Transmission through a thin film) or, using the experimental data from such an experiment, if can determine the complex refractive index of the thin film.

2 Installation

To install RefDex on your computer, download and run the installer. Administrator status will be required to install RefDex. Follow the instructions in the installion wizard, this will involve downloading resources from the Mathworks website required to run RefDex.

RefDex can take a significant time to start up, especially on older systems. Do not assume that because the program window did not appear yet, that it is not currently starting up.

3 User Interface

This section will describe how to use the user interface of RefDex.

3.1 Toolbar

The toolbar consists of the menus **File**, **Options**, **Advanced** and **Help**.

3.1.1 File

Pressing on the **File** button reveals the options **Open**, **Save**, **Save As** and **View**. **Open** opens a file browser to find the correct file to be opened in RefDex. This is typically used to open raw nk data which has been previously saved to disc. By default RefDex searches for files with the extension ".txt", however you can also choose to search for all file types. Note that a correct file format is formated into three columns, optional column headers are allowed. The first column is always the wavelength in nanometers. The second and third columns are either R/T, Psi/Delta or n/k. **Save** will save the contents of the last succesfully completed calculation to disc. If an output filename has not been selected then this button will function the same as **SaveAs**. **SaveAs** opens a file browser to find the desired folder to save the calculation data. Additionally a name for the output data must be given, the default file extesion is ".txt" however this can be changed by typing in a different extension. **View** will show the currently loaded results (either R/T, Psi/Delta or n/k data) as a function of wavelength. **Load Settings** and **Save Settings** can be used to open and save to disc the current RefDex main window settings. **Exit** will close all open RefDex windows including the program itself.

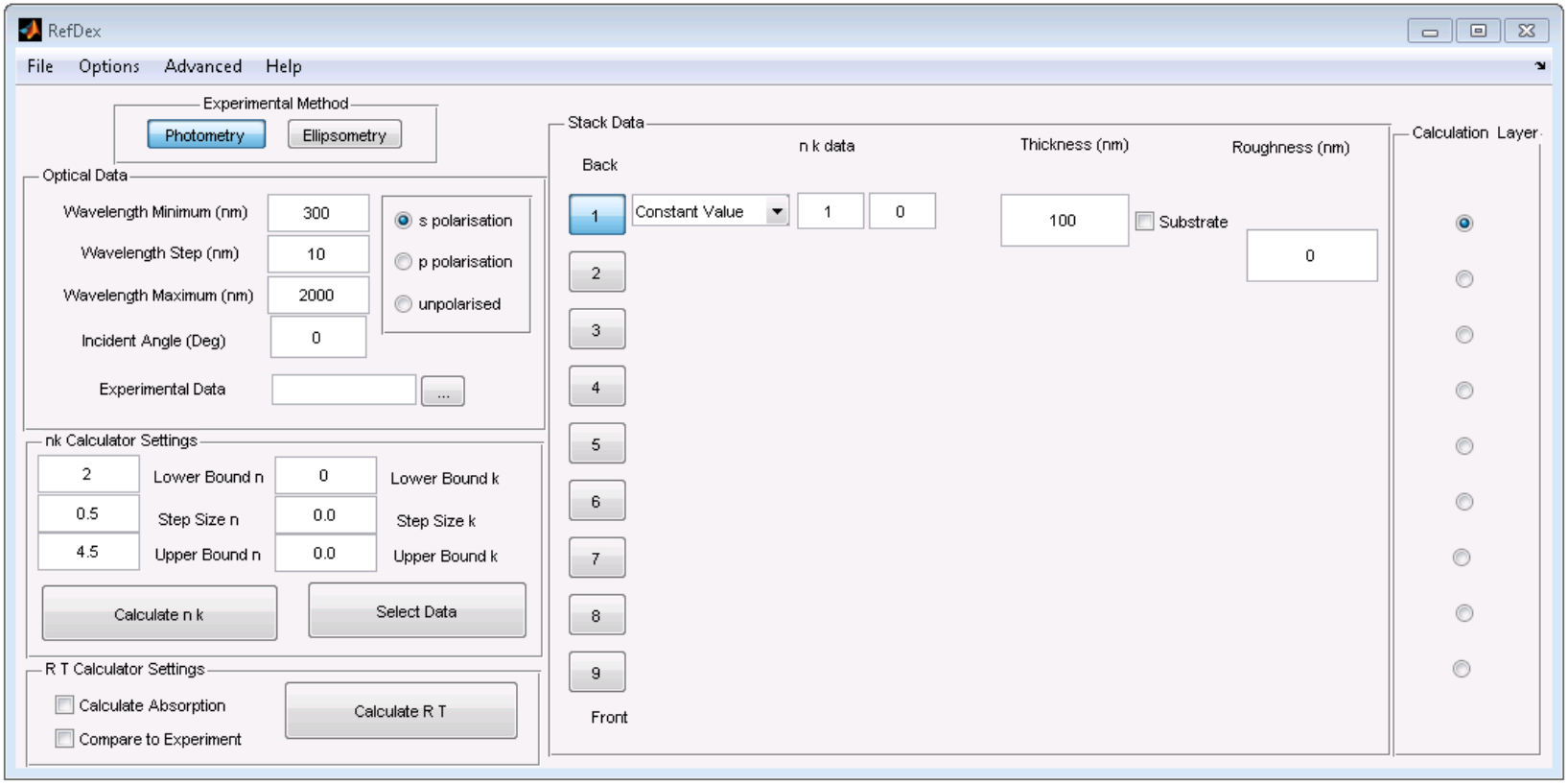

Figure 3.1: The RefDex main interface.

3.1.2 Options

Photometry Units determines the units of calculated reflection and transmission spectra, also the units that input reflection and transmission data should have. Unitary means $0 < R, T < 1$ whilst percent means $0 < R, T < 100$. **Absorption Layers** sets the layers which will be displayed after a calculation of the absorption. Note that the absorption is always calculated in all layers, this just sets which layers are displayed. **Substrate Averaging** sets the method used for dealing with incoherent layers (typically substrates). the default option "Intensity Coupling" is quicker, however it cannot provide accurate results for the absorption when including substrate layers (reflection, transmission and nk calulcation are correct). Therefore the option "Phase Averaging" can be chosen which calculates also the absorption correctly for incoherent layers, but takes longer to calculate.

3.1.3 Advanced

The options contained in **Advanced** are all further options for either RT, $\Psi\Delta$ or nk calculations. As such their uses are described in the relevant sections.

3.1.4 Help

Pressing **Help** will attempt to open this pdf document, requires a valid pdf reader to be installed on the computer. **About** will bring up a box giving the details of the current version of RefDex, press "okay" to close the box.

3.2 Experimental Method

The toggle switch moves between photometry (i.e. reflection / transmission) and ellipsometry modes. This means that in photometry mode, the reflection and transmission can be calculated, furthermore the n and k of a thin film can be calculated using reflection and transmission measurements as an input. For more information about photometry mode see section 4 Likewise in ellipsometry mode the ellipsometric paramters Psi (Ψ) and Delta (Δ) will be calculated, furthermore the n and k of a thin film can be calculated using Ψ and Δ measurements as an input. For more information about ellipsometry mode see section 7

3.3 Optical Data

This section groups together the input parameters of a calculation which relate to the optics.

3.3.1 Wavelength

The input boxes **Wavelength Minimum**, **Wavelength Step** and **Wavelength Maximum** determine the wavelengths which will be used for the calculation in nanometers. The wavelengths used for the calculation run from **Wavelength Minimum** to **Wavelength Maximum** in steps of **Wavelength Step**.

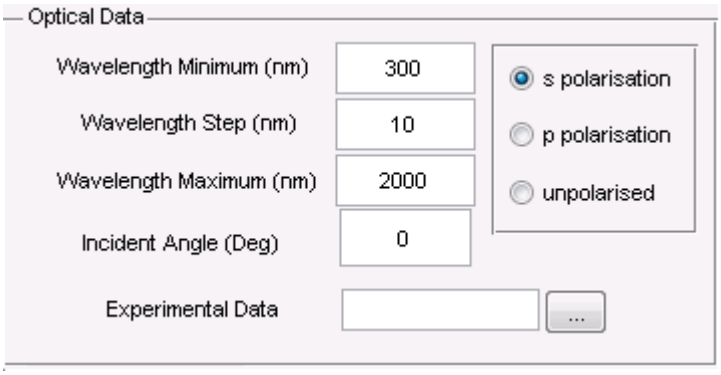

Figure 3.3: Optical data user interface

Wavelength	nanometers
Reflection	unitary (percentage)
Transmission	unitary (percentage)
Psi	-180 to $180°$
Delta	-180 to $180°$

Table 3.3.1: The units for the experimental input data. Units for reflection and transmission can optionally be changed to percentage, see section 3.1.2

3.3.2 Angle

The input box **Incident Angle** will determine the incident angle of the light into the thin film stack in degrees. After the usual convention, an angle of 0 means that the light is perpendicular to the plane of the thin film. For the case of a reflection / transmission calculation it is possible to choose the polarisation of the incident light, the options are s, p and unpolarised (50:50 mix of the s and p results) light. Note that for an incident angle of 0, all three will give identical results. Note that this is unavailable for ellipsometry calculations due to ellipsometry requiring both the s and p polarised reflection to calculate Ψ and Δ.

3.3.3 Experimental Data

The text box allows the user to give the path to input exprimental data (reflection/transmission or psi/delta) which has been saved on the computer. Pressing the (...) button next to the text box will allow the browsing of files and folders on the computer. By default RefDex searches for .txt files but this can be changed to all files in the browser. The format for input data should be a 3xN list giving the Wavelength in the first column followed by the relevant experimental values in the second column. The first row can be text labels for the columns. RefDex will automatically recognise if the columns are tab, comma or space separated. The units for the different values are given in table 3.3.3. If surface roughness or inhomogeneous layers are implimented, measured reflection and transmission data should be specular not total. For more information see appendix C

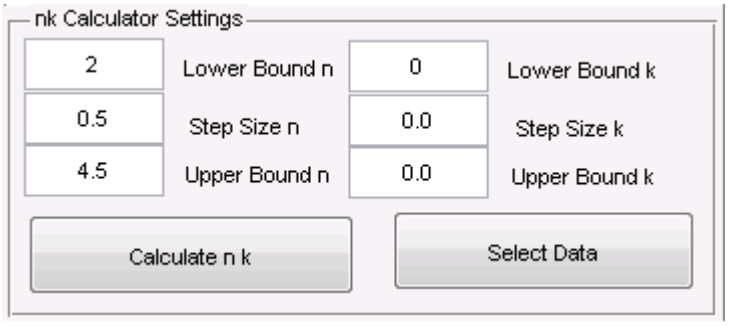

Figure 3.4: nk calculator settings user interface

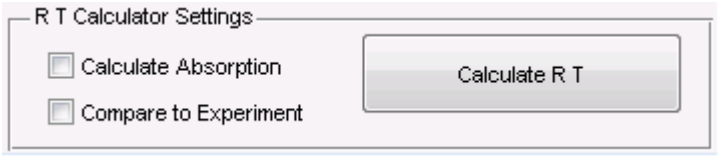

Figure 3.5: RT calculator settings user interface

3.4 nk Calculator Settings

This section contains inputs for the nk calculator and related functions. The uses of setting bounds for an n and k calculation are discusses in more detail in section 5. The n values will run from **Lower Bound n** to **Upper Bound n** in steps of **Step Size n**, likewise for k values. The button **Calculate n k** will start an calculation of the refractive index of the layer selected in the **Calculation Layer** 3.7 section. When the results of a refractive index calculation are in the RefDex memory, either by first completing a refractive index calculation or by loading previous results using 3.1.1, the select data will allow for the interactive selection of a physically meaningful solution of the n k data. For more information on the data selection process see section 6.

3.5 R T (Psi Delta) Calculation Settings

The push button **Calculate R T** will calculate the reflection and transmission of the thin film stack defined in 3.6. If the calculation mode is set to ellipsometry this button will instead calculate the Psi and Delta values. If **Compare to Experiment** is selected, then the calculation will be compared to the R and T or Psi and Delta values input in 3.3.3. If calculation mode is set to photometry then the the absorption in the layer stack can be calculated by selecting **Calculate Absorption**. The calculation of absorption may differ strongly from reality for highly scattering systems.

3.6 Stack Data

This section describes the physical parameters of the multilayered stack which is under investigation.

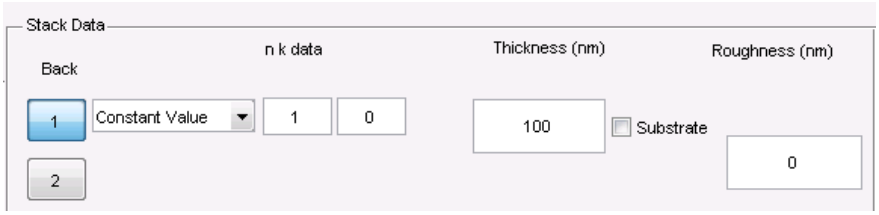

Figure 3.6: stack data user interface

> The front of the sample will be the layer with the higest number, i.e. layer 3 is more towards the front than layer 2.

Select the amount of layers desired by pressing the numbered buttons 1-9 on the left hand side of this section. RefDex does not required that layers be selected in order, e.g. a calculation can be performed with layers 1,2,4,5 selected and layer 3 deselected. This can be used to turn on/off layers inside the multilayer stack without rearranging all the layers. For each layer the physical properties must be defined:

3.6.1 nk Data

The dropdown menu allows to choose from the different methods of inputing the n and k data. Selecting **Constant Value** means that the n and k for this layer will be constant with respect to wavelength over the whole wavelength range. The default setting of $n = 1$ and $k = 0$ describes air and should be used for the first and last layer in the stack. By choosing the option **From File**, the n and k data can be uploaded from a text file. Either type the file path directly into the text box, or click on the (...) box to browse for the correct file on the computer. The text file shoud contain a 3 x N array with the columns being wavelength (nm) followed by the n and k value at that wavelength. Make certain that there are n and k values for at least two different wavelengths, that no wavelength is repeated, and that the wavelengths in this file span the range of wavelengths for the calculation chosen in 3.3.1. The file may have text column headers.

3.6.2 Thickness, Substrate, Roughness

The **Thickness** of the layer should be given in nanometers. For very thick films (i.e. substrates) it may be convenient to use scientific notation, i.e. $1e6$ instead of 1000000 to represent a 1mm thick substrate (in nanometers). The thickness is only important for layers in the film stack. The first and last layers will typically be air, which is outside the film stack and the thickness plays no role, therefore it can safely be left at the default value of 100 nm. Check the box **Substrate** if the layer is thick compared to the coherence length of the light and therefore should be modeled incoherently. For practical purposes this will be the substrate upon which the thin film(s) is deposited. The **Roughness** is the rms roughness of the boundary between the layer and the next layer below. The roughness is implemented using the scalar scattering theory, more information can be found in Appendix C.

Surface roughness is only compatable with photometry (not ellipsometry) mode at normal incidence. Additionally this will result in a calculation of the specular reflection and transmission, for a discussion of the difference between specular and total reflection and transmission see Appendix C.

3.7 Calculation Layer

This section is used to choose which layer will be labelled as the calculation layer. When performing an n and k calculation this will be the layer for which the n and k values are calculated. When using the advanced feature **Inhomogeneous Layer** in both n and k calculation and reflection / transmission calculation, this will be the layer which is modelled inhomogeneously, for more information see section 9. When using the advanced feature **Effective Medium** in both the n and k, reflection / transmission and ellipsometric calculation, this will be the layer where the effective medium is applied.

4 Reflection and Transmission Calculation

This section will describe how to use the reflection and transmission calculator. For information on how to set the indivdual input parameters, see section 3

1. Make sure that the experimental method is set to photometry.
2. Input the wavelengths for which you would like to calculate the reflection and transmission. Note that a larger wavelength range or a smaller step size may increase the calculation time required.
3. (Optional) Input the incident angle of the the light and the polarisation.
4. (Optional) If comparing to an experimental reflection and transmission, give the path to the data and click the **Compare to Expriment** box.
5. Input the stack data. Pressing the numbered buttons 1-9 will activate or deactivate the layer. Typically the first and last layer should be left with the default settings (n=1,k=0, thickness=100, roughness =0) to simulate the air surrounding the film stack. All other layers need at least the thickness and the refractive index to be defined. When loading the refractive index from file, make sure that the wavelength range of the refractive index data spans the wavelength range selected for the calculation.
6. (Optional) Define which layers are substrate layers.
7. (Optional) Input the surface roughness of layers.
8. (Optional) If using advanced features, select which layer they should be applied to using the calculation layer selection.

9. (Optional) If calculating the absorption in each layer, click the **Calculate Absorption** box.
10. Click on **Calculate R T** to begin the calculation.

After the calculation is finished, the calculated reflection and transmission spectra will appear as a graph on the screen. To save the graph as an image, choose **File** and **Save** in the image window. To save the wavelength / reflection / transmission as a .txt data file, go back to the RefDex main window and choose **File** and **Save** there.

4.1 Absorption Calculation

Calculating the absorption provides a stacked plot of absorption in each layer plus the reflection and transmission. It is possible to exclude displaying the the absorption in certain layers by deselecting the layers in **Options** > **Absorption Layers**. Note that the absorption is always calculated in all layers, this option just changes which layers are displayed. To save the graph as an image, choose **File** and **Save** in the image window. To save the wavelength / reflection / transmission / absorption as a .txt data file, go back to the RefDex main window and choose **File** and **Save** there.

> Currently absorption calculation is not compatable with incoherent layers (i.e. transparent substrates).

5 Refractive Index Calculation

This section will describe how to use the refractive index (nk) calculator. For information on how to set the indivdual input parameters, see section 3

1. Choose either photometry or ellipsometry depending on what experimental data have been taken.
2. Input the wavelengths for for you would like to calculate the n and k. Note that a larger wavelength range or a smaller step size may increase the calculation time required.
3. Input the incident angle at which the measurement was taken at, if reflection transmission was used, input the polarisation used (unneccesary for incident angle = 0).
4. Give the path to the experimental data.
5. Input the stack data. Pressing the numbered buttons 1-9 will activate or deactivate the layer. Typically the first and last layers should be left with the default settings (n=1,k=0, thickness=100, roughness =0) to simulate the air surrounding the film stack. All other layers need at least the thickness and the refractive index to be defined. When loading the refractive index from file, make sure that the wavelength range of the refractive index data spans the wavelength range selected for the calculation. The refractive index does not need to be defined for the layer where the refractive index will be calculated (i.e. n and k can be left on the default settings).
6. (Optional) Define which layers are substrate layers.

7. (Optional) Input the surface roughness of layers.
8. Select which layer will be the calculation layer (i.e. the layer in which the n and k will be calculated).
9. Input the lower, upper bound and step size for the n and k. This is explained in detail below.
10. Click the **Calculate n k** button.

As the calculation runs, each value of n and k will be appended to a graph, when the progress bar disappears the calculation is complete. After the calculation is finished, the calculated n and k spectra will appear as a graph on the screen. To save the graph as an image, choose **File** and **Save** in the image window. To save the wavelength / n / k as a .txt data file, go back to the RefDex main window and choose **File** and **Save** there. It is highly recommended to save the n k data to file before moving to the **Data Selection** stage.

5.1 Bounding of n and k

When calculating the n and k data, RefDex searches for the n and k values which give the closest match of the simulated optical data to the experimental optical data. For more details see appendix B. In order to do this, a starting value for the n and k are required. The bounding value tells RefDex the value of n and k to start searching at. Due to the fact that different values of n and k can lead to the same value for R and T or Psi and Delta, it is necessary to start the search for n and k at many different points. This ensures that all values of n and k which give the correct optical data are found. Therefore the n and k bound are both a range of values. As an example, if the n bound is set to vary from 1.5 to 2 in steps of 0.5 and the k bound varies from 0 to 1 in steps of 1, RefDex will first search (at each wavelength) for the correct n and k value beginning with n = 1.5 and k =0. After this the calculation will be repeated for n = 2, k = 0. Then again the calculation will be performed twice more for n = 1.5, k =1 and n = 2, k = 1. The values for the n and k bound may be difficult to choose and rely on the user knowing a ballpark figure for the n and k value of the sample. If no information about the n k data is known, it is recommended to first use a rough calculation that begins at many n and k values which are widely spread. The results of this calculation will reveal the approximate n and k value which can be used for another calculation with the n and k bound more focused. To create a smooth data set from the calculated n and k data we refer to the data selection section 6

6 Data Selection

If there is n k data in the RefDex memory, either because an n k calculation has completed or because data has been loaded in the RefDex main window, pressing on the **Select Data** button will open the data selection window. The idea of the data selection window is to fit a smooth curve to the calculated n and k data.

6.1 Controls

The toggling of n and k changes currently viewed data in the plot axis. To begin fitting the data click on the **Place Vertices** button. The mouse cursor will change to a crosshair, this crosshair can be used to place vertices onto to spectrum of n or k data. The following controls apply when placing vertices:

1. By left clicking on the graph a new vertex will be placed.
2. By right clicking the placement of vertices will be paused.
3. To restart vertex placement, right click on any vertex and select "restart vertex placement".
4. When vertex placement is paused the indivdual vertices can be moved to different positions by holding left click and dragging the vertex.
5. When vertex placement is paused the entire vertex structure can be moved to a different position by holding left click and dragging on a line between vertices.
6. When vertex placement is paused, new vertices can be added inbeween existing vertices by holding CTRL+A and left clicking on the line joining two vertices.
7. When vertex placement is paused, vertices can be deleted by right clicking on a vertex and selecting "delete vertex".

When the vertices have been placed, pause the placement of vertices and click on **Fit**. This will interpolate the placed vertices with a smooth (piecewise cubic) curve. If the fit is not adequate the placement of vertices can be restarted by click on **Place Vertices** again. If a fit exists for either the n or k values, when looking at the raw data for the other value (e.g. when looking at the k values if a fit exists for the n values) certain values will be highlighted. These are the values which are the pair values to those lying closest to the fit line for the other value. For example, when a fit exists for the n values, when viewing the k values, the k values will be highlighted which are the pair values of the n values which lie closest to the fit for the n values. In this case, pair value means that a value of n and k are always calculated together in a "pair", therefore if one value is selected as physically meaningful the its pair value should also be chosen. The benefit to highlighting values comes when one of the n or k has a clear physically meaingful solution, but the other value does not. A fit can then be made to the physically meaningful data, and then for the other data, those values can be chosen which correspond to the physically meaningful solution.

When a fit has been made for both the n and k values, clicking on **Save and Exit** will close the window and put the fitted solution into the RefDex memory. This can then be saved to file using **File** and **Save As** (using Save As will avoid saving over the raw data used to generate the fit).

7 Ellipsometry Mode

When using elliposometry mode most of the actions taken will be the same as those taken when using photometry mode. Things that should be noted

in ellipsometry mode:

1. Psi and Delta values should are calculated, and should be given as an input in the format -180 to $180°$.
2. It is crucial to set the incident angle correctly.
3. roughness and inhomogeneous layers are not implimented for ellipsometry mode, usage of these features in ellipsometry mode will give erronious results.
4. it is not possible to calculate the absorption when in ellipsometry mode.

8 Effective Medium

This section will describe the usage of the advanced feature **Effective Medium**. To use this feature simply click on Effective Medium in the **Advanced** drop down menu, this will open the effective medium window.

8.1 Use Effective Medium

Click on the **Use Effective Medium** button to apply the effective medium to the layer marked as "calculation layer" in the RefDex main interface.

8.2 Effective Medium Type

Select the desired type of effective medium from the dropdown menu. Types available are volume fraction, Maxwell-Garnett and Bruggeman. For more information on the different types of effective medium see D.

8.3 Material Data Path

The path to the refractive index data for the the inclusion material should be given in the text box. Press the (...) button to browse the computer file system for the specific path. The data format should be a 3xN array with columns wavelength (nm), n and k. This material will form an effective medium using the refractive index data for the layer labelled "calculation layer" in the RefDex main interface.

8.4 Effective Medium Fraction

Enter the volume fraction of the effective medium.

> Certain effective medium approximations are only valid for certain volume fractions (i.e. Maxwell-Garnett assumes small volume fraction, whereas Bruggeman assumes high volume fraction).

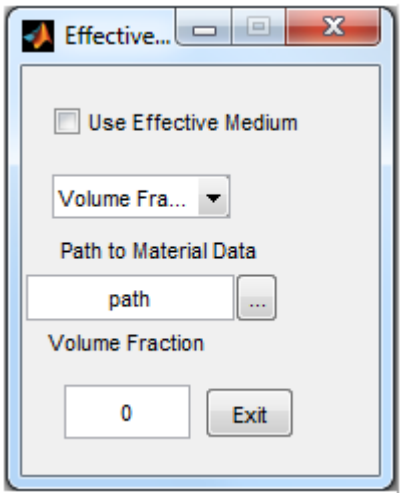

Figure 8.1: Effective medium user interface

9 Inhomogeneous Layer

This section will describe the usage of the advanced feature **Inhomogeneous Layer**. To use this feature simply click on Inhomogeneous Layer in the **Advanced** drop down menu, this will open the inhomogeneous layer window.

9.1 Toolbar

The toolbar consists of the menus **File** and **Advanced**.

9.1.1 File

Pressing on the **File** button reveals the options **Open**, **Save** and **Save As**. **Open** opens a file browser to find the correct file to be opened. Only the results of previous 3D distribution calculations which have been saved to disc may be loaded. **Save** will save the contents of the last succesfully completed 3D distribution calculation to disc. If an output filename has not been selected then this button will function the same as **SaveAs**. **SaveAs** opens a file browser to find the desired folder to save the calculation data. Additionally a name for the output data must be given.

9.1.2 Options

Options gives the option to change the isosurface output from **view 3D Distribution** to a negative version. The negative version will display the voids as particles floating in free space, as opposed to the default option of showing a film containing voids.

9.2 Interface

Check the box **Calculation Layer Inhomogeneous** to activate the inhomogeneous layer for the RefDex calculation. In order for this to work both an inhomogineity distribution and a 3D distribution have to be defined.

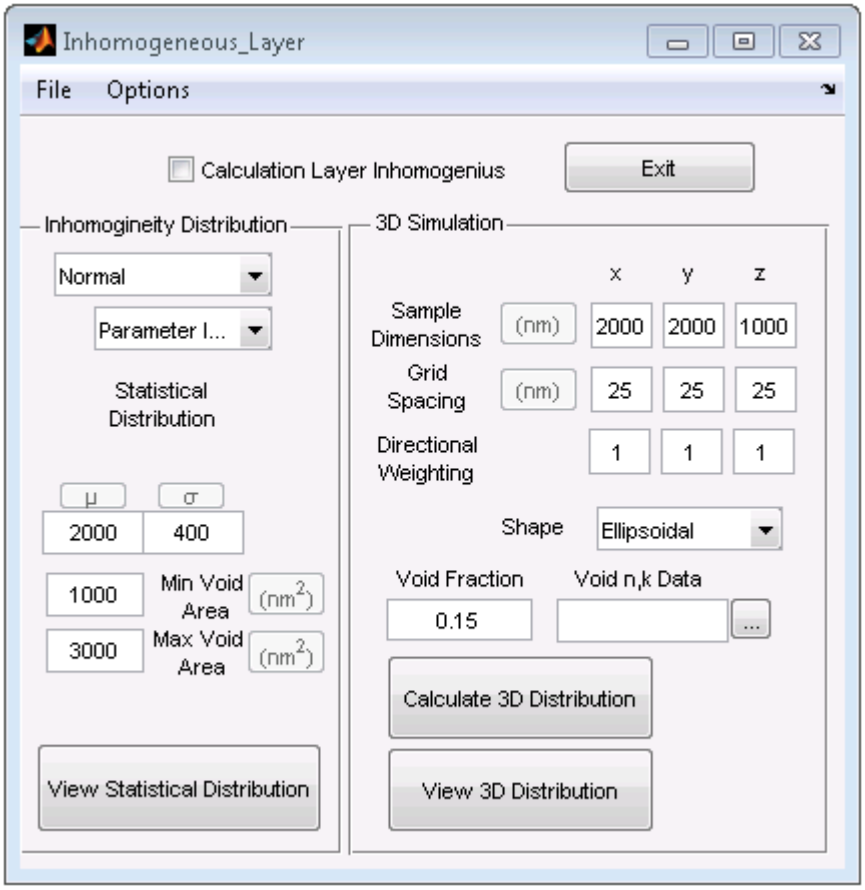

Figure 9.1: Inhomogeneous layer user interface

9.3 Inhomogineity Distribution

This section is used to define the statistical distribution of the voids on the top surface of the inhomogeneous layer. There are two methods to define the distribution, it can either be fit to experimental data, or input directly. To change between the two methods of input select the desired method from the second drop down menu. When the the relevant inputs have been given, click on **View Statistical Distribution** to generate and view the statistical distribution, the distribution is then ready to use for the 3D simulation section.

9.3.1 Statistical Distribution

The first drop down menu is used to choose the type of statistical distribution, the choices are Normal, Exponential, Log Normal, Pareto and Bounded Pareto. For more background on these distributions see appendix F.

9.3.2 Parameter Input

If parameter input has been selected then two statistical parameters must be given to define the distribution (e.g. for Normal distribution these are mean and standard deviation) for details on these parameters see appendix F. Additionally the minimum and maximum void area in squared nanometers must be given.

9.3.3 Experimental Distribution

If experimental distribution is selected then a text box appears to input the path to experimental data. Use the (...) box to browse for the file on the computer. The file should be a .txt file consisting of a 1xN array containing the areas of the surface voids in square nanometers. This kind of data can be obtained by taking a picture of the sample and using an image processing tool to calculate the sizes of the voids on the picture.

9.4 3D Simulation

The 3D simulation section uses the statistical distribution of surface voids supplied by the previous section to generate a 3D distribution of the voids inside the layer. A set of auxillary statistics are then extracted from this 3D simulation which is used directly in the RefDex calculation. When the correct inputs have been given, clicking on **Calculate 3D Distribution** will calculate the 3D distribtuon and **View 3D Distribution** will visualise it. The visualisation shows the top surface, side surface, a contour map of the void distribution in the x-y plane and an isosurface showing the film with the voids inside.

9.4.1 Sample Dimension

The sample dimension describe the size of the inhomogeneous film in the x y and z directions. Values should be given in nanometers.

9.4.2 Grid Spacing

The 3D simulation is performed on a cuboidal grid. Smaller values for the grid spacing will provide a higher resolution 3D simulation are the expense of computational time and memory requirements.

9.4.3 Directional Weighting

The weighting determines how elongated the voids will be in certain directions. This can be useful for the case of anisotropic voids.

9.5 Shape, Void Fraction, Void n,k Data

The **Shape** determines the primitive used to describe the voids. Ellipsoidal voids are quick to generate and flexible enough for most cases. Random voids start with a seed point on the grid and randomly add more points to the surface until the volume is reaches that determined by the surface statistical distribution. The **Void Fraction** is the volume fraction of the voids, this can be estimated by measuring the surface coverage of voids. **Void n,k Data** allows the uploading of n k data to describe the material of the voids. If this is left empty then the voids are assumed to be air.

A Transfer Matrix Method

The transfer matrix method is used to calculate the forwards and backwards propagating electric fields in a stack of perfectly smooth homogeneous films. For reflection and transmission the intensity is the required quantity, which can be obtained from the square of the electric field. For ellipsometry the ratio of the reflected beams for different polarisations is the important factor. In order to calculate the electric fields, we begin with a vector containing the forwards and backwards electric field strength at on one side of the thin film,

$$\begin{pmatrix} E^+ \\ E^- \end{pmatrix}, \tag{1}$$

We then act upon this vector using two different matrices. The dynamical matrix describes how the field changes when changing from one medium to another,

$$\begin{pmatrix} E_i^+ \\ E_i^- \end{pmatrix} = \frac{1}{t_{i,j}} \begin{pmatrix} 1 & r_{i,j} \\ r_{i,j} & 1 \end{pmatrix} \begin{pmatrix} E_j^+ \\ E_j^- \end{pmatrix}, \tag{2}$$

where the well known Fresnel coefficients are,

$$r_{i,j} = \frac{n_j \cos\theta_i - n_i \cos\theta_j}{n_j \cos\theta_i + n_j \cos\theta_j}, t_{i,j} = \frac{2n_j \cos\theta_i}{n_j \cos\theta_i + n_j \cos\theta_j}. \tag{3}$$

For propagation inside the layer, we apply the propagation matrix,

$$\begin{pmatrix} E_i^+ \\ E_i^- \end{pmatrix} = \begin{pmatrix} \phi_i^{-1} & 1 \\ 1 & \phi_i \end{pmatrix} \begin{pmatrix} E_i^+ \\ E_i^- \end{pmatrix}, \tag{4}$$

$$\phi_i = e^{-\imath \frac{2\pi}{\lambda} n_i d_i} \tag{5}$$

where λ is the wavelength of the light, n_i is the complex refractive index of the layer i and d_i is the thickness of layer i.

By iteratively applying dynamical and propagation matrices the electric field at each side of the layer stack can be linked,

$$\begin{pmatrix} E_1^+ \\ E_1^- \end{pmatrix} = \frac{1}{t_{1,2}} \begin{pmatrix} 1 & r_{1,2} \\ r_{1,2} & 1 \end{pmatrix} \begin{pmatrix} \phi_2^{-1} & 1 \\ 1 & \phi_2 \end{pmatrix} \cdots \\ \cdots \begin{pmatrix} \phi_{N-1}^{-1} & 1 \\ 1 & \phi_{N-1} \end{pmatrix} \frac{1}{t_{N-1,N}} \begin{pmatrix} 1 & r_{N-1,N} \\ r_{N-1,N} & 1 \end{pmatrix} \begin{pmatrix} E_N^+ \\ E_N^- \end{pmatrix}.$$

When modelling the outcome of a reflection transmission measurement we impose the conditions that the electric field incident on the front surface $E_1^+ = 1$ and that there is no light incident on the rear side $E_N^- = 0$. In doing so we can identify $E_1^- = r$ and $E_N^+ = t$, where r and t are the amplitude reflection coefficients for the layer stack. Finally to obtain the reflection and transmission we use,

$$R = |r|^2, T = \frac{\cos\theta_1}{\cos\theta_n}|t|^2. \tag{6}$$

B Refractive Index Calculation

A provides a model for R and T in terms of the thicknesses and complex refractive indices of the layers in the stack. Using this it is possible to "reverse" the equation. Consider if R and T are known, and in addition the thicknesses of all film layers, and the complex refractive index of all layers apart from one. By guessing values for n and k for the unknown layer and comparing the resulting calculated R and T to the experimentally, it is possible to obtain the n and k of the unkown layer. Mathematically we seek the values of n and k which minimise,

$$\left(R_{calc}(n,k) - R_{exp}\right)^2 + \left(T_{calc}(n,k) - T_{exp}\right)^2. \tag{7}$$

Unfortunatly this is not a unique minimisation, that is, different n,k value pairs can minimise this equation. Only one of these pairs will be the physically meaningful solution. Therefore it is necessary for the user of RefDex to decide which values of n,k are physically meaningful. To decide which values are physically meaningful, the following guidelines may be helpful.

1. Apart from meta-materials, the n value of a sample will be non-negative.
2. Non metallic layers will have an n value greater than 1.
3. Transparent materials should have a k value very close to zero (in their transparent region).
4. For dielectric and semiconductors not at a resonance (i.e. an absorption band) the n value will vary slowly with the wavelength and will show normal dispersion (i.e. increasing n value with decreasing wavelength).

The efficacy of this method depends on the accuracy of the transfer matrix model. For cases which deviate from the assumptions made by the transfer matrix method (smooth, homogeneous layers) it may be necessary to envoke corrections to the standard trasfer matrix method. These are the surface roughness, effective medium and inhomogeneous layer techniques outlined in appendices C and E.

C Scalar Scattering Theory

The scalar scattering theory of Beckmann and Spizichino provides a way to describe the specular R and T at normal incidence coming from a rough interface. When light is scattered out of the specular direction due to the interface roughness, the reflection and transmission Fresnel coefficients of that interface are reduced. This means when comparing R and T calculated with this theory to experimnent, the experimental value must be both specular and at normal incidence. To obtain the specular reflection and transmission, one can measure the total and diffuse reflection and transmission, then use the relation $R_{Spec} = R_{Total} - R_{Dif}$. The new Fresnel coefficients are given by,

$$r_{i,j}^{'} = r_{i,j} \exp\left[-2\left(2\pi n_i \frac{\sigma}{\lambda}\right)^2\right] \quad (8)$$

$$r_{j,i}^{'} = r_{j,i} \exp\left[-2\left(2\pi n_j \frac{\sigma}{\lambda}\right)^2\right] \quad (9)$$

$$t_{i,j}^{'} = t_{i,j} \exp\left[-\frac{1}{2}\left(2\pi (n_i - n_j) \frac{\sigma}{\lambda}\right)^2\right] \quad (10)$$

$$t_{j,i}^{'} = t_{j,i} \exp\left[-\frac{1}{2}\left(2\pi (n_j - n_i) \frac{\sigma}{\lambda}\right)^2\right], \quad (11)$$

where σ is the rms roughness of the surface, n_i is the complex refractive index of layer i and lambda is the wavelength of the light.

D Effective Medium

In some cases, an inhomogeneous layer may be well described by a so called effective medium which uses some basic assumptions to combine the refractive index data of two different materials into a single medium. The types of effective medium implimented in RefDex are:

D.1 Volume Fraction

The volume fraction approximation simply mixes the n and k of the two materials after the volume fraction of each,

$$n_{eff} = w_h n_h + \sum_i w_i n_i k_{eff} \qquad = w_h k_h + \sum_i w_i k_i, \quad (12)$$

where w_h and w_i are the volume fractions of the host material and ith inclusion. Likewise n_h and n_i are the refractive indices of the host material and ith inclusion. This approximation, whilst simple to understand and implement, has no physical basis and therefore should be used with caution.

D.2 Maxwell Garnett

The Maxwell Garnett approximation assumes spherical particles distributed sparesly inside a host matrix so that the field felt by each particle is independent of the other particles. Using this and basic electrostatics, one comes to the equation,

$$\left(\frac{\epsilon_{eff} - \epsilon_h}{\epsilon_{eff} + 2\epsilon_h}\right) = \sum_i w_i \left(\frac{\epsilon_i - \epsilon_h}{\epsilon_i + 2\epsilon_h}\right). \quad (13)$$

Due to the assumption for a sparse distribution, the volume fraction of inlusion materials w_i should be small. If that is the case, the Bruggeman approximation may be better suited.

D.3 Bruggeman

The Bruggeman approximation assumes spherical particles (or grains) of two types of material randomly distributed but closely packed together. It is then considered that each particle feels the effect of an effective medium made up of all the other particles. This selfconsistancy condition and again the use of elementary electrostatics produces the equation,

$$w_h(\frac{\epsilon_h - \epsilon_{eff}}{\epsilon_h + 2\epsilon_{eff}}) = -w_i(\frac{\epsilon_i - \epsilon_{eff}}{\epsilon_i + 2\epsilon_{eff}}). \tag{14}$$

Due to the assumption that each particle feels the effect of both materials (i.e. the effective medium) the volume fraction w_i of the inclusion should not be small (¡0.1). If that is the case, the Maxwell Garnett approximation may be better suited.

E Inhomogeneous Calculation

During a calculation using an inhomogeneous layer, the aim is to model the 3D distribution of voids inside the layer. RefDex will then take this distribution and extract the necessary statistics to perform transfer matrix calculations. To get the distribution accurate it is recommended to compare to an image of the sample which is being simulated. Things to consider when calculating the 3D distribution are:

1. The distribution will become more accurate for a larger simulated x-y plane, this comes at the cost of calculation time and computer memory.
2. It is recommended to keep the grid spacing the same in all directions to avoid artifacts which can occur for larger discrepancies between the spacings.
3. Each void which is placed will undergo a rotation to randomise orientations. The primitive will be rotated by $0 < \phi < 2\pi$ around the z axis and by $-\pi/4 < \theta < \pi/4$ around the x and y axes.

F Statistical Distributions

This appendix describes the various statistical distributions used in the inhomogeneous layer advanced feature.

1. Normal distribution described by the mean μ and standard deviation σ.
$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/(2\sigma^2)} \tag{15}$$
2. Exponential distribution described by a single parameter λ.
$$P(x) = \lambda e^{-\lambda x} \tag{16}$$

3. Log-Normal distribution described by the mean μ and standard deviation σ.

$$P(x) = \frac{1}{x\sigma\sqrt{2\pi}} e^{-(\ln x - \mu)^2/(2\sigma^2)} \tag{17}$$

4. Pareto distribtuon defined by two parameters α and x_m.

$$P(x) = \frac{\alpha x_m^\alpha}{x^{\alpha+1}} \text{ for } x \geq x_m \tag{18}$$

5. Bounded Pareto distribtuon defined by three parameters $\alpha > 0$,$L > 0$ and $H > L$.

$$P(x) = \frac{\alpha L^\alpha x^{-\alpha-1}}{1 - (\frac{L}{H})^\alpha}. \tag{19}$$

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