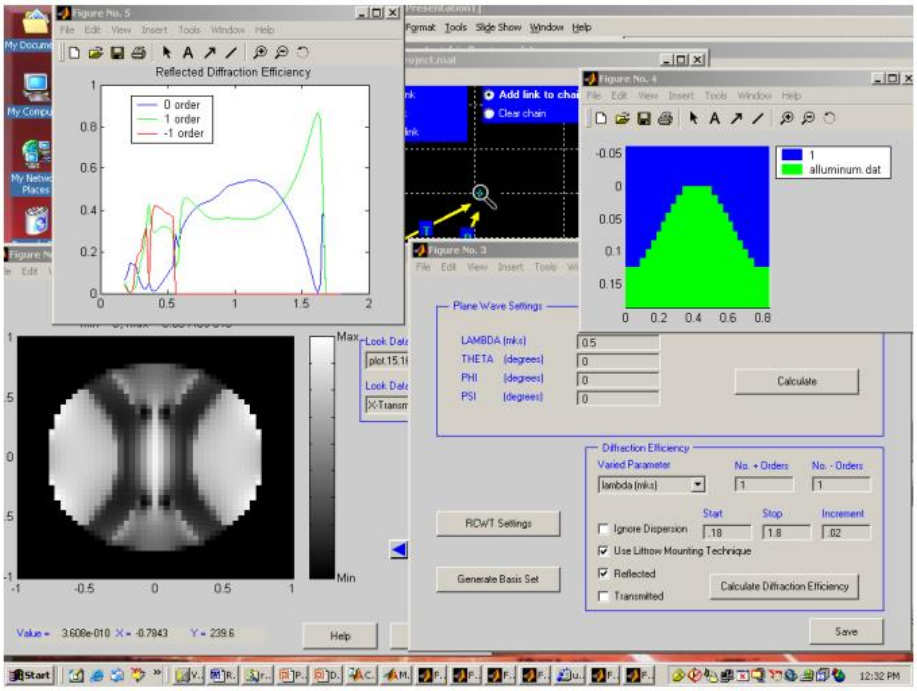
The Optiscan RCWT calculator



Contents:

1. Introduction:

The Optiscan rigorous coupled wave theory (RCWT) package was developed to incorporate a powerful method of rigorously simulating diffraction grating structures into the Optiscan simulation engine. This document serves as a guide to using this powerful computational tool. It is assumed that the user of this software package is familiar with basic diffraction theory (especially the angular spectrum representation of an optical field), as well as basic Fourier theory. The RCWT calculator has three primary functions. It calculates the reflected and transmitted electric fields which result from an arbitrary plane wave incident on the grating structure. It can calculate the diffraction efficiency of a grating structure as a function of several variables. And finally it can be used to generate a basis set for mapping an arbitrary incident electric field to the fields reflected from, and transmitted through the grating structure. The first two of these three capabilities are, while powerful, are simple and straightforward to use. However, the basis set calculation (the most powerful capability of the RCWT package) is a rather complex calculation and requires a substantial amount of care to set up correctly. Consequently a large portion of this manual is devoted to it's use.

Section 2 of this manual presents a mathematical background of the RCWT algorithm. In order to use the RCWT package to it's full potential, some familiarity with this background is understandably necessary. Section 3 gives an overview on using the RCWT calculator in Optiscan. This section discusses every aspect of the RCWT calculator, except the basis set generator. Section 4 discusses how to use the basis set calculator in Optiscan, and presents two examples (which are included with the Optiscan distribution). The mathematical details involved in the basis set calculation are also presented in this section.

2. Background:

Rigorous coupled-wave theory (RCWT) is a rigorous solution to Maxwell's equations for a plane wave incident on a physical, possibly many layered, structure that is infinite in extent and periodic in one dimension, with a period Λ.[1,2,3]

The basic principle behind RCWT is that a complex structure is divided into several layers, and the permittivity variation of each layer is expressed as a Fourier series. Furthermore, electric and magnetic fields, above and below the structure, as well as within each layer, are also expressed as a Fourier series of plane waves. The base frequency of each of these plane waves is determined by applying the Floquet condition (also referred to as the grating equation) given by

$$k_{xj} = k_0 \left[n_I \sin\theta - j \frac{\lambda_0}{\Lambda} \right]$$

where n_I is the complex index of the incident material, θ is the angle of the incident plane wave, Λ is the period of the permittivity variation and j is an indexing integer (not an imaginary number). This condition forces each layer to have the same base period, or be uniform. However the permittivity modulation can be arbitrarily complex within the basic period Λ.

Both the electric and magnetic fields in each layer of the structure are represented as a Fourier series, using the same set of plane waves. Application of Maxwell's equations to this representation results in a coupled set of differential equations, which are solved using an eigenvalue/eigenvector approach. Once this eigenvalue problem is solved, boundary conditions are applied at each interface of the structure. Application of these boundary conditions results in a set of algebraic coupled linear equations, which are solved using a straightforward matrix technique. However, a direct inversion of these linear equations can result in numerical stability problems. Fortunately these problems have been addressed, and the solution is easily implementable.[2]

RCWT is only one of several methods that can be used to rigorously analyze the systems considered in this dissertation. Other methods include, finite difference methods[4], and complex field summation methods[5].

The accuracy of the RCWT method is determined by the number of orders kept in the truncated series used to express the permittivity and the electric field spectrum.

2.1 What RCWT can do:

RCWT accurately solves the Mawell's equations for a linear media in which the permittivity variation can be expressed as a multiply layered binary structure. RCWT is best suited for Binary grating structure, however, complex structures, such as cosine gratings and blazed gratings are approximated by layering binary structures. RCWT is particularly well suited to dealing with dielectric materials. Metals can also be accurately simulated.

While the RCWT algorithm was originally developed to calculate the diffraction efficiency of binary grating structures, it can also be used to directly calculate the electric fields reflected from and transmitted through the structure. This capability extends the applicability of RCWT to calculate the effect of a grating structure on an arbitrary electric field. The electric field incident on the surface of the grating structure is decomposed into an angular spectrum of plane waves for each of the standard x,y and z polarization states. The incident angular spectrum is transformed into s-type and p-type polarization states. The RCWT algorithm is then applied to the s and p polarization components of each incident plane wave. The results of each of these calculations are a spectrum of s-type and p-type wavefronts. The s-type and p-type spectra are recombined and transformed to x,y, and z polarization states.

As a demonstration of the accuracy of the Optiscan RCWT package, the results of Reference 8 are reproduced in Example 2 in section 4.3 of this manual. In the experiment performed in Reference 8, a collimated x-polarized (or y-polarized) electric field is focused onto a cosinusoidal gold (n=0.23+i*3.2) diffraction grating using a 0.8 numerical aperture objective lens. The period of the structure is 0.60 μm and the depth is 0.15 μm. The cosine profile is approximated using five binary layers and is shown in figure 1. The reflected irradiance in the exit pupil of the objective lens is calculated and shown in figure 13 for both x and y incident polarization states. These results can be compared directly to the results shown in Figures 4 and 7 of Reference 8, which show both measured and calculated (using a different method) data for the physical system being simulated.

2.2 Problems with RCWT:

Two factors determine the accuracy of the RCWT algorithm, the number of orders kept in the truncated series representing the electric field (and the media permittivity), and binary layering used to simulate the structure. In the limit of an infinite number of orders and layers, results in an exact solution to Maxwell's equations. However, the number of orders required to achieve an accurate solution differs depending on the problem in question. The minimum number of orders required for any configuration is 2*d/lambda where d is the base period of the structure. Therefore, large period structures, require a large number of orders and therefore, longer computation times. In general, for dielectric media, the minimum number of orders is often sufficient. However, for metal structures, a large number of evanescent orders are required to achieve an accurate result. RCWT is known to handle s-type (TE) polarization much better than p-type (TM) polarization, which generally requires a larger number of orders (although this difficulty is greatly reduced by using the reciprocal permittivity technique given by Lalanne and Morris in Ref. 3.

There is also an inherent instability in the basic RCWT algorithm**. This instability occurs when using a non-periodic layer (such as an air-gap), if the base period times the index of the layer is exactly equal to an integer times the wavelength.** This problem occurs because the algorithm attempts to invert a matrix, which is singular. As long as physical values for refractive index are used this instability is unlikely to be a problem, except in the case of an air gap. When this situation occurs using a value of 1.00029 (the true index of refraction of air) will result in a stable solution.

3. Using the RCWT calculator in Optiscan:

3.1 Grating structure definition:

Many simulationsl begin by defining the physical structure of the diffraction grating being analyzed. The parameters in the grating structure are completely up to the user. That is, any structure that can be constructed using a stack of binary layers can be simulated using the Optiscan RCWT calculator. Thin film stacks can also be included simply by setting the two indices in a given layer to the same value. However, it should be kept in mind that the minimum number of orders used in the RCWT algorithm is 2*d/lambda. Therefore, it must be emphasized that large period grating structures, will require a large number of orders and will likewise require a large calculation time. Also note that a large number of layers will also increase the calculation time.

To define a grating:
1. In the main RCWT calculator panel, click "RCWT settings" to open the RCWT settings window.

2. Input the base period of the grating, keeping in mind that the minimum number of orders required for a calculation is 2d/lambda.

3. Input the complex index of refraction for the incident media and the substrate. If you plan on performing wavelength dependent calculations, you will likely want to use a dispersion file. The dispersion file is a tab delimited ASCII text file in which the first column is wavelength in microns, the second column is the real part of the complex index and the third column is the imaginary part of the complex index. The format for the dispersion file is:

1.23450000000000	1.21200000000000	12.46400000000000
1.12227272727273	1.20100000000000	11.18100000000000
1.02875000000000	1.26000000000000	10.01000000000000
0.94961538461538	1.46800000000000	8.94900000000000
0.88178571428571	2.23700000000000	8.21200000000000

Optiscan will automatically interpolate between the discrete values given in the data file

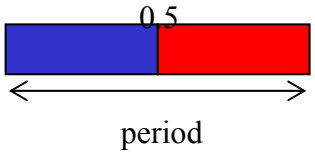
4. Click on the "RCWT Layers" Tab to begin defining the layers of your grating

5. Use the "New Layer" button to add as many layers is required for your desired grating structure.

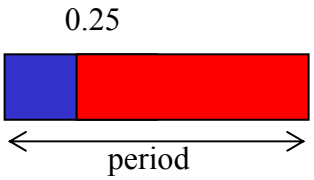
6. The height is the thickness of the layer.

7. Input the two index values that define the modulation of your grating structure. If desired, you can use a dispersion file for each index. If you want to use an unmodulated layer, you simply set Index 1 and Index2 to the same value.

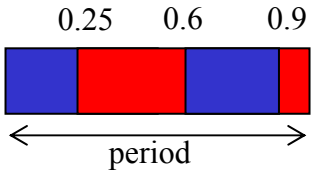
8. Define the duty cycle vector for the layer. The values in the duty cycle vector are sequential values between zero and one that define the transition points between Index 1 and Index 2. For example



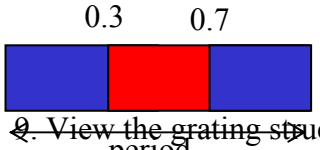
Duty cycle vector = 0.5



Duty cycle vector =0.25



Duty cycle vector = [0.25 0.6 0.9]



Duty cycle vector =[0.3 0.7]

9. View the grating structure using the preview button.

Example: A 1-micron deep cosine grating with a 1-micron period

Layer number	Height	Index 1	Index 2	Duty cycle vector
1	0.2	1.0	Aluminum.dat	0.39758 0.60242
2	0.2	1.0	Aluminum.dat	0.31549 0.68451
3	0.2	1.0	Aluminum.dat	0.25 0.75
4	0.2	1.0	Aluminum.dat	0.18451 0.81549
5	0.2	1.0	Aluminum.dat	0.10242 0.89758

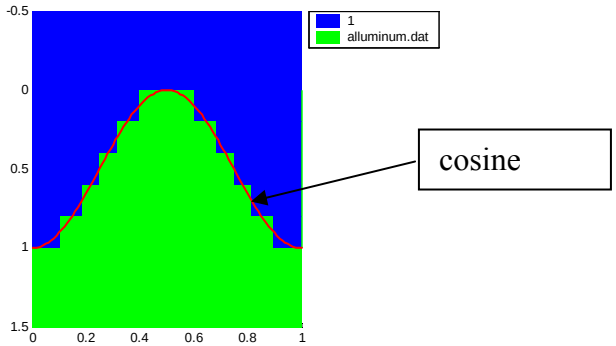


Figure 1

3.2 Number of orders.

The number of orders required to achieve an accurate result from the RCWT calculator is dependent on three factors.

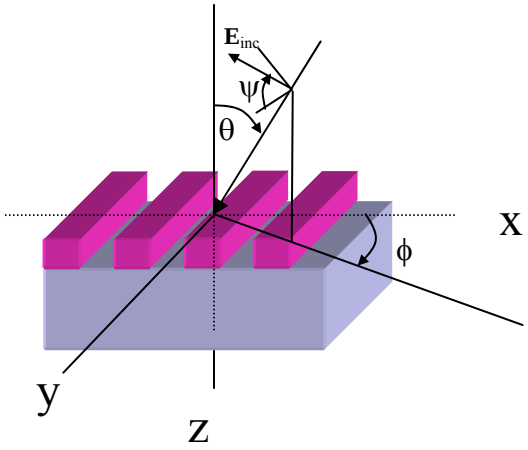
1. The period of the grating: The minimum number of orders is 2*d/lambda.
2. The material being used: For dielectric materials, the minimum number of orders is generally sufficient, although it is often a good idea to include at least a few orders above the minimum. For metals, more orders are required, especially with P-type polarization, to account for any plasmon and surface wave effects. Generally with metal structures, a good place to start is twice the minimum number of orders. For materials in which the imaginary part of the complex index is high (above 1) even more orders will likely be required.
3. Number of layers: Generally structures with several layers require a few more orders than single surface structures.

Obviously the user wants to minimize the number of orders required to produce an accurate result. The best way to determine the correct number of orders is to perform a diffraction efficiency calculation for p-type polarization and increase the number of orders until the answer stops changing.

3.3 Simple Electric field calculator

Once the grating structure has been defined, the transmitted and reflected electric fields can be easily calculated in terms of the four parameters in the main window. Lambda is the wavelength of the illuminating electric field. The three angles define the plane wave that is incident on the grating.

θ is the angle of incidence with respect to the z-axis
ϕ is the rotational angle about the z-axis
ψ is the polarization angle 90^o= s-polarization 0^o=p-polarization.



The values set in these boxes are also used as base values for the diffraction efficiency calculator.

The E-field calculator is extremely useful in basic grating design, because it allows for a quick check of the grating structure properties. For example consider the somewhat complicated grating design given by

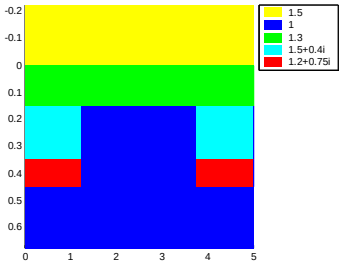


Figure 2

This structure could easily represent something like a phase shifting mask used in microlithography. The complex layer structure does not allow for a simple analysis of the transmission properties. However, the basic electric field calculator will generate the transmitted electric field for easy analysis.

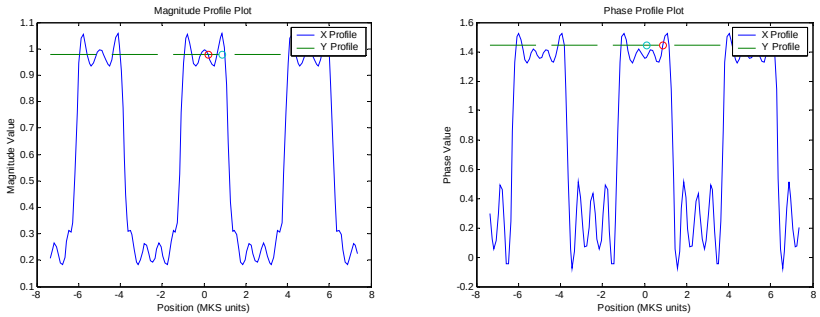


Figure 3

3.4 Diffraction Efficiency calculator.

Because RCWT was primarily developed for measuring diffraction efficiency, Optiscan has obviously included this capability in the RCWT calculator. Using the efficiency calculator is straightforward. The user simply selects the parameter they wish to vary using the "Varied parameter" pull down menu, and selects the range and sampling of the data required. All other parameters are taken from the "Plane wave Settings" Panel. For example, in the following configuration the rotational angle phi is 10^o and the polarization angle is 45^o . The incident angle theta is varied from 0^o to 89^o in 5^o increments.

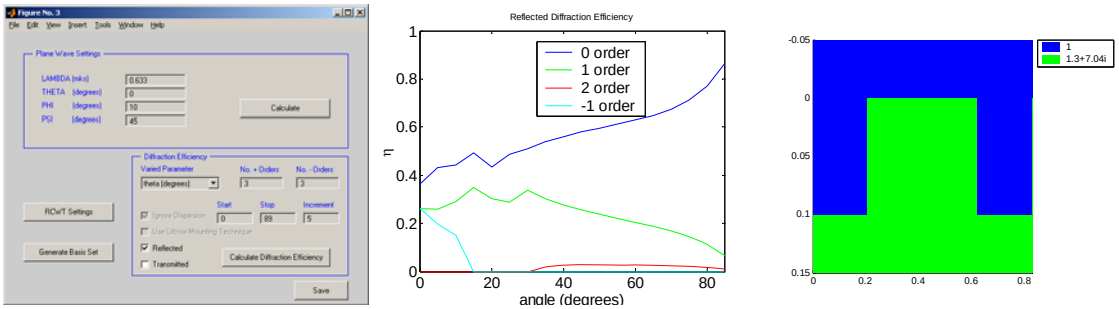


Figure 4

If the user chooses to vary the parameter of wavelength, two additional options are allowed. Firstly, the user can choose to ignore the effects of dispersion (the change in refractive index with wavelength). This option is not normally recommended, unless the user does not have available refractive index data, and the range of wavelengths is rather small. The second option allows the user to calculate the diffraction efficiency as a function of wavelength, assuming the grating is in a first order Littrow mount. A first order Littrow mount is designed such that the first diffracted order propagates backwards, nearly parallel to the beam illuminating the grating. These mountings are used extensively in spectroscopy because it gives the maximum diffraction efficiency as a

function of wavelength. When using a Littrow mount, the change in wavelength is coupled to a change in incident angle through the relationship

$$2\sin\theta_i = \frac{\lambda}{d}.$$

Therefore, when the Littrow mounting box is checked and the "theta" parameter in the "Plane wave settings" panel is equal to zero, then the first diffracted order reflected from the grating, is parallel to the incident wave. If the theta parameter is 8^o then there is an 8^o difference between the incident beam and the beam reflected back from the grating. Figures ?? show the diffraction efficiency as a function of wavelength from a cosine grating structure in a first order Littrow mount for p-type polarization. The data is shown1200 ln/mm (0.833 μm period), aluminum gratings with a depth of 0.1245 μm (h/d=0.15). The cosine pattern is approximated by 10 layers. These diffraction efficiency results can be compared to the efficiency data given in chapter 4 of Reference [11]

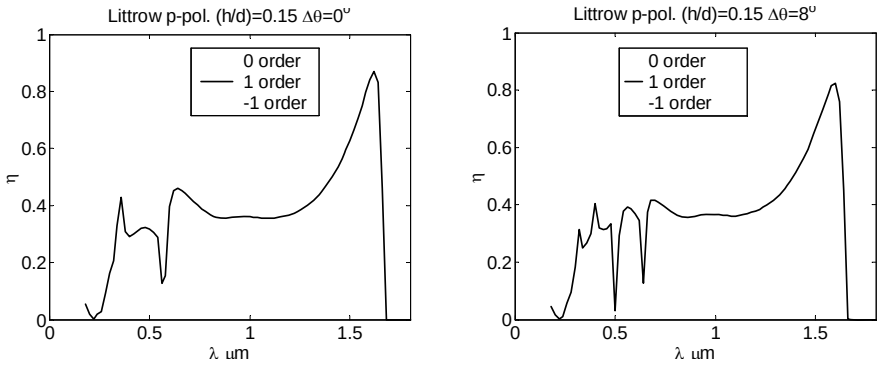


Figure 5

4. Basis set generator

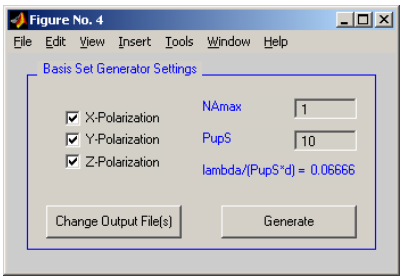
The primary feature in the Optiscan RCWT calculator is the RCWT Basis set generator. This capability allows the RCWT calculator to interface directly with the optical system modeling capability of Optiscan.

The purpose of the RCWT basis set generator is to provide a method of calculating the electric field reflected from or transmitted through a grating given an arbitrary incident electric field. The basic principle behind this procedure is that the incident electric field is decomposed into a collection of plane waves. Each of these plane waves interacts with the grating structure producing a reflected spectrum of plane waves. The spectra produced by all the incident plane waves are added together, producing the angular spectrum of the electric field reflected from the structure. However, this procedure can be extremely time consuming for situations in which reasonably fine spectral sampling is required. For example, if the angular spectrum requires a cross sectional sampling of say 50 pixels, then approximately 2500 RCWT calculations are required, for each state of incident polarization. Therefore, to calculate the interaction with an arbitrary vector electric field approximately 7500 RCWT calculations are required. If each RCWT calculation requires 2 seconds to complete, the

complete analysis requires more than 4 hours. However, when performing optical modeling, it is advantageous to be able to change the physical properties of the incident field, and calculate the reflected (transmitted) field is a very timely fashion. In order to accomplish this, the RCWT basis set calculator calculates the reflected spectra from a unit amplitude spectrum for and incident x,y and z state of polarization. The results of this calculation are then stored, and used as a basis set, which can be used to transform any incident electric field, simply by properly scaling, and assembling the stored reflected spectra. Therefore, provided the physical properties of the grating structure do not change, only one time-consuming calculation is required to incorporate the grating structure into the optical modeling of Optiscan. Optiscan simply uses the precalculated basis set to recalculate the electric field reflected from (transmitted through) the grating as various optical system parameters, such as defocus, incident polarization etc. are changed.

4.1 Generating a basis set:

To generate a basis set, the user begins by defining the grating structure to be used. This includes the wavelength, number of orders and the base period. *The user will probably want to determine the optimum number of orders using the diffraction efficiency calculator ,before calculating a basis set.* Once the diffraction grating has been defined, click on the "Generate Basis Set" button. When this occurs, the following box appears



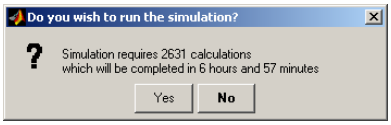
The user then selects the polarization of the input electric field. If the polarization of the incident electric field changes with position (such as with a High NA focused spot) the user should select all three polarization states. When generating the basis set, there are two additional parameters that are required by the user. The most important of these parameters is the PupS value. The PupS variable is an integer fraction of the angular spectrum sampling of the reflected wavefront. This means that the spectral sampling of the output wavefront is given by

$$\Delta(n_1\alpha) = \frac{\lambda}{(d \cdot \mathrm{PupS})}$$

where n_1 is the index of the incident media, λ is the wavelength, d is the base period of the grating and PupS is an *integer* defined by the user. This relationship is required by the RCWT algorithm. For a complete basis set, the number of calculations required for all three polarization states is roughly

$$N \approx \pi\left(\frac{PupS \cdot d}{\lambda}\right)^2 \times 3$$

The length of time required for each calculation is determined by the computer processor speed, number of orders chosen, and the number of layers in the grating structure. When the user clicks on "Generate" the computer does one timed calculation and estimates the time required to generate the complete basis set. A window "pops up" Telling the user how long the calculation will take and asks the user if they wish to continue. The length of time required is highly dependent on the system being simulated and can range from several minutes to several hours.



If the user wishes to simulate a low numerical aperture system, often times a very fine angular sampling, over a small angular spectrum might be required. However, in order to achieve this fine angular sampling, the PupS parameter must be set to a very large number. This presents a problem, because the calculation time increases quadratically with an increase in PupS.
If the system is a low-NA system, a complete basis set calculation is unlikely to be required. The user can limit the basis set calculation by specifying the NAmax parameter. By specifying the NAmax parameter, the user limits the range of angles that are calculated for the basis set. (note the NAmax parameter is really the maximum direction cosine value)

4.2 The PupS parameter.

PupS is used to determine the spectral sampling of the output field. The spatial sampling of the electric field generated using the RCWT algorithm is determined solely by the number of orders and the grating period. This sampling is given by

$$\Delta x = d/(2*(m+1))$$

where m is the number of orders (actually the number of positive orders, which is half the total number of orders). Therefore, the electric field representing a unit cell of the grating has N0=2*(m+1) sample points. The spectral sampling for a data set given by a single unit cell of the structure is given by

$$\Delta\alpha = \lambda/(N0*\Delta x) = \lambda/d,$$

which is precisely the sampling given by the Fouquet condition. For small period gratings, this angular spectral sampling is often too coarse. However, the spectral sampling is improved by simulating multiple unit cells of the grating structure. In this case, the data set representing the electric field has PupS*N0 data points, where PupS is an integer representing the number of unit cells being simulated. In this case, the spectral sampling is given by

$$\Delta\alpha = \lambda/(N0*PupS*\Delta x) = \lambda/(d*PupS),$$

The Optiscan RCWT calculator works by mapping the spectra of the incident electric field to the spectra of the output electric field. Therefore, it is required that the spectral sampling of the input electric field be given by

$\Delta\alpha=\lambda/(d*PupS)$.

In order to insure that this condition is met, Optiscan interpolates the spectrum of the input electric field into an array with this sampling. Therefore, PupS should be chosen such that $\lambda/(d*PupS)$ is as close to the sampling of the input electric field in order to minimize any errors that result from the linear interpolation. For example, consider an incident electric field is a Gaussian beam, in a 256x256 point array with a sampling given by $\Delta x=0.25$ μm and $\lambda=0.633$μm. The spectral sampling of the input field is therefore, given by

$\Delta\alpha_{input}=\lambda/(N_x*\Delta x)=0.633/(256*0.5)=0.0099$

Assuming the grating structure of interest has a period of 2 μm, then PupS should be chosen to be

$PupS=\lambda/(d*\Delta\alpha)=.633/(2*.0099)=32$

This means that if the number of orders is chosen to be the minimum of m=2*d/lambda=7, then the output electric field is an array of PupS*(2*m+1)=480 points on a side. Notice that the size of output array will increase as the number of orders is increased. Say for example, the grating is metal, and 21 orders are required for a stable solution then the output array has 1376 points on a side. However, since Optiscan works primarily in the spectral domain, and only the propagating spectral components are mapped (for now), the output spectra is a $1/\Delta\alpha$ x $1/\Delta\beta$ array (200x200 in this case) representing the angular distribution of the field diffracted by the grating. Often times this is the only output that is required. However, if the near field data is necessary, the output spectra can be mapped back to the near field using an inverse Fourier transform. Note that the evanescent components of the resultant electric field are included in the spectral mapping (although they are of course included in the RCWT calculation).

If the user wishes to analyze near field effects, which require the inclusion of evanescent waves, an air gap can be added to the unit cell definition of the grating structure. This is illustrated below

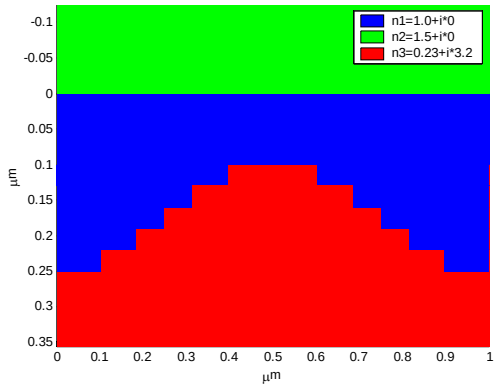


Figure 6

Note, one can also use the air gap to simulate defocus effects.

4.3 Using the Basis Set in Optiscan:

Included with the Optiscan RCWT calculator is the preprogrammed function

[OutPup]=RCWTpupMAP(InPuP,FILES);

which is uses the RCWT basis set data and allows easy incorporation of the RCWT basis set calculation into Optiscan, by using the MOP operator. The InPuP variable is a Matlab structure of the form

InPuP.PXin= angular spectrum of the x-polarization of the incident electric field
InPuP.PYin= angular spectrum of the y-polarization of the incident electric field
InPuP.PZin= angular spectrum of the z-polarization of the incident electric field

InPuP.avecin=a vector whose elements represent the coordinate axis $n_1\alpha$
InPuP.bvecin=a vector whose elements represent the coordinate axis $n_1\beta$

Ideally the sampling of the input angular spectrum should be $\lambda/(d*PupS)$ where d is the period of the grating. However, Optiscan will interpolate the the coordinates into the correct sampling.

The OutPup variable that the function returns is also a Matlab structure of the form

OutPup.PxR=angular spectrum of the x-polarization of the reflected electric field
OutPup.PyR= angular spectrum of the y-polarization of the reflected electric field
OutPup.PzR= angular spectrum of the y-polarization of the reflected electric field

OutPup.PxT=angular spectrum of the x-polarization of the transmitted electric field
OutPup.PyT = angular spectrum of the y-polarization of the transmitted electric field
OutPup.PzT = angular spectrum of the y-polarization of the transmitted electric field

OutPup.avec=a vector whose elements represent the coordinate axis $n_1\alpha$ sampled at $\Delta(n_1\alpha)=\lambda/(d*PupS)$

OutPup.bvec=a vector whose elements represent the coordinate axis $n_1\beta$ sampled at $\Delta(n_1\beta)=\lambda/(d*PupS)$

Ideally the spectral sampling for the angular spectrum arrays in the InPup structure and the OutPup structure should be the same, that is $\Delta(n_1\alpha)=\lambda/(d*PupS)$. However, the function RCWTpupMAP will interpolated the spectral sampling of the InPup structure into the correct sampling. Nevertheless, the user should make an effort to insure the sampling interval of the incident field is reasonably close to the ideal interval of $\Delta(n_1\alpha)=\lambda/(d*PupS)$.

Recall that the spectral sampling is given by $\Delta(n_1\alpha)=\lambda/(d*PupS)$. This can be somewhat confusing since most of the values entered in an Optiscan simulation are spatial positions or physical distances. Because most of the calculations done in Optiscan are based on the discrete Fourier transform algorithm (actually the fast Fourier transform algorithm), the relationship between spectral coordinates and spatial distances is given by

$$\Delta(n_1\alpha)= n_1\lambda/(N\,\Delta x).$$

where $\Delta(n_1\alpha)$ is the spectral sampling Δx is the spatial sampling and N is the number of elements in the array representing the spatial electric field.

Finally, the FILES input is a structure that contains the location of the

FILES.fnameX=string specifying the path of the x-polarized basis set data
FILES.fnameY=string specifying the path of the y-polarized basis set data
FILES.fnameZ=string specifying the path of the Z-polarized basis set data

4.4 Examples:

Be aware that the RCWT basis set generator calculation is an extremely sophisticated, and somewhat complicated simulation and that the proper choice of simulation values is critical to the success of the calculation. Furthermore, because the basis set calculation can be extremely time consuming, the user is **strongly encouraged** to spend some time planning the desired simulation before beginning the Optiscan calculation. The user should have a good idea of the grating period and both the spatial and spectral (ie NA, or angular extent) dimensions of the incident, transmitted and reflected electric fields. The user should keep in mind that **changes to the parameters of the diffraction grating, or the spectral sampling of the basis set require a completely new basis set calculation**, and therefore must be chosen carefully.

Example 1: *Importing an electric field*

The RCWTpupMAP function can be used once the RCWT calculator has been used to calculate the RCWT basis set. The Optiscan SOURCE object can be used to construct an incident electric field such as x-polarized Gaussian beam waist.

The basic layout for the simulation is shown below. The SOURCE object creates the incident electric field, then a MOP object uses the RCWTpupMAP function to transform the electric field.

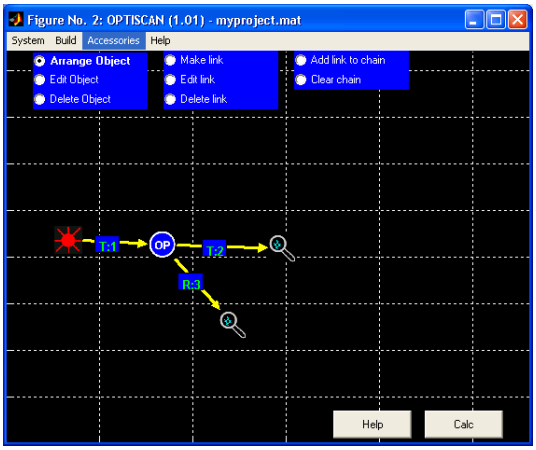


Figure 7

The first step is to PLAN THE CALCULATION. Say that a nominally 2 micron Gaussian spot is incident on a dielectric binary (in this case) diffraction grating (n=1.5) with a period of 1.600 microns and that the wavelength is 633nm. A 2 micron Gaussian spot at l=633nm produces an electric field with a spectral range of about α_{max}=0.316 (0.633micron/2microns=0.316). Assume that we wish to sample the calculated spectra with an interval of $\Delta\alpha$=0.06 (roughly 10 points across the angular spectrum of the zero order of transmitted (or reflected) beam). Therefore, the value of PupS should be chosen to be 7 (λ=0.633 /[$\Delta\alpha$=0.06 * d=1.6]). With this value chosen for PupS, the number of calculations required is roughly π*(1/ $\Delta\alpha^2$) or 800 calculations, for each polarization.

Once this planning stage is done, a source is defined in optiscan that represents the electric field at the surface of the grating structure. If the user wants a spectral sampling of $\Delta\alpha$=0.06 then the spatial sampling of the incident field must be chosen such that

$\Delta x = \lambda/(N\ \Delta\alpha)$.

Assuming that the user wants to use a reasonable array size of 255 pixels then the resultant spatial sampling is approximately .042 microns (this number does not have to be exact, Optiscan will interpolate the results correctly, however is should be reasonably close to minimize any errors involved with interpolation).

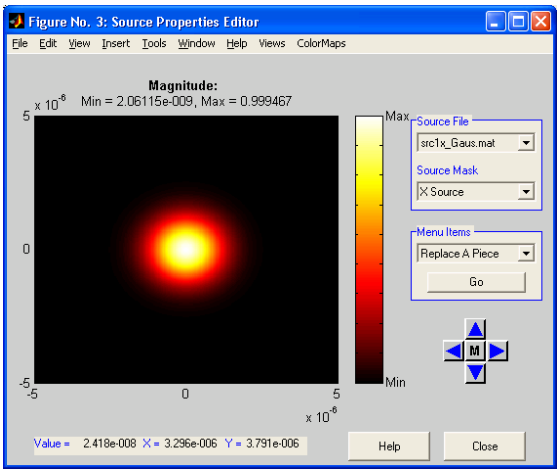


Figure 8

Now that the calculation has been planned and the source defined, the user defines the grating structure using the predetermined parameters (Grating period=0.8 microns, lambda=0.633 microns and PupS=7). The minimum number of order for this calculation is 2d/lambda≈3 (although a number like 10 is probably more reasonable. Use the diffraction efficiency calculator to determine the optimum value for this.)

Next, the electric field generated by the source object is imported into a MOP (Mathematical Operation) object which performs the RCWT mapping calculation.

An example MOP script for importing an electric field from a source object and calculating the electric field reflected and transmitted from the grating structure is as follows

```
function [mop, curlink, simdata, errmsg] = mymop(action, mop, curlink, simdata)

    errmsg = '';

Ex=simdata.Ext;

 xvec=simdata.sysxvec;
 yvec=simdata.sysyvec;
 lambda=simdata.LAMBDA;


xsamp=abs(xvec(2)-xvec(1));
ysamp=abs(yvec(2)-yvec(1));
NX=length(xvec);
NY=length(yvec);
```

```
InPuP.PXin=fftshift(fft2(fftshift(Ex)))/(NX^2);
InPuP.PYin=zeros(size(Ex)); %no y polarization component
InPuP.PZin=zeros(size(Ex)); %no z-polarization component

InPuP.avec=[-NX/2:NX/2-1]*lambda/(NX*xsamp);
InPuP.bvec=[-NX/2:NX/2-1]*lambda/(NX*ysamp);

FILES.fnameZ=fullfile(mop,'<project>\<userdata>\','RCWTdataZ');
FILES.fnameX=fullfile(mop,'<project>\<userdata>\','RCWTdataX');
FILES.fnameY=fullfile(mop,'<project>\<userdata>\','RCWTdataY');

[OutPup]=RCWTpupMAP(InPuP,FILES);

PxR=OutPup.PxR;
PyR=OutPup.PyR;
PzR=OutPup.PzR;

PxT=OutPup.PxT;
PyT=OutPup.PyT;
PzT=OutPup.PzT;

avecout=OutPup.avec;
bvecout=OutPup.bvec;

%update the source fieds
simdata.Exr= PxR;
simdata.Eyr= PyR;
simdata.Ezr= PzR;
simdata.sysxvec=avecout;
simdata.sysyvec=bvecout;

simdata.Ext = PxT;
simdata.Eyt = PyT;
simdata.Ezt = PzT;
```

The first step in this script is to import the data from the source object, and to calculate the position sampling intervals for the imported data. Next, the electric fields are converted to angular spectra, using a fast Fourier transform operation (FFT), and spectral position vectors (avecin and bvecin) are calculated for the spectral data. Note that the positional sampling in the source definition is chosen such that the sample spacing in the spectral position vectors is (lambda/(PupS d)) where d is the grating period and PupS is chosen in the basis set calculation panel *before the basis set is calculated*. The command

```
[OutPup]=RCWTpupMAP(InPuP,FILES);
```

Performs the RCWT calculation and OutPup is a MatLab structure which contains the propagating spectral data of the electric fields transmitted and reflected from the structure. Note that evanescent fields are not contained in the output data (although they are used in the RCWT calculation) . If near-field effects are desired, they should be included in the geometry of the structure used to calculate the basis set.

Once the MOP calculation is completed, a LOOK object is used to view the simulation result. Note that the x and y coordinates in the electric field are direction cosines and not spatial coordinates.

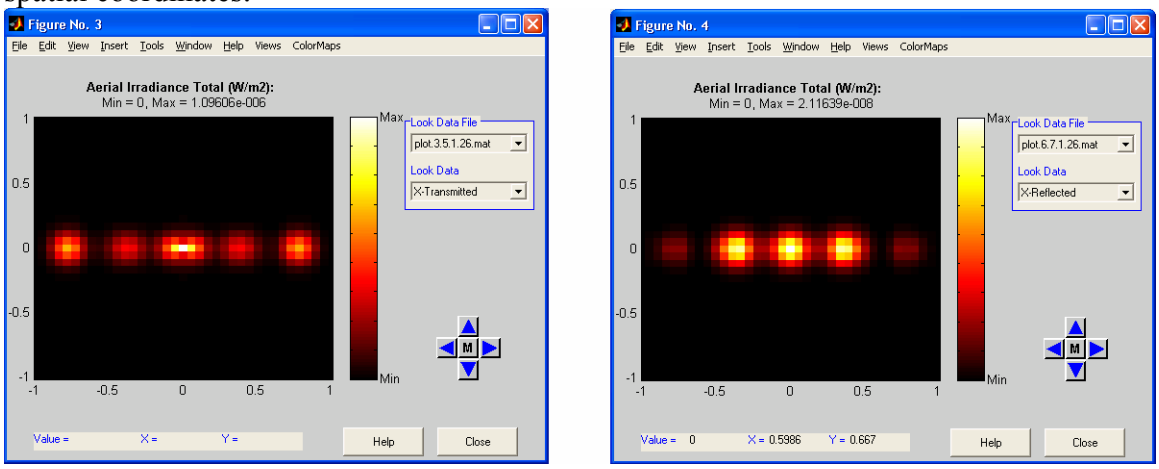


Figure 9

Example 2: *Incorporating an optical system*

Often times the electric field incident on the grating structure is not known, and must be simulated using Optiscan. This example demonstrates a full-vector calculation of a focused spot using the Optiscan LENS object. The user begins be defining a source (in this case a Gaussian spot) . Next the source is linked to a optical element. For this example a high NA 7x ideal system with an image space NA of about 0.75 is used (although any lens system can be used).

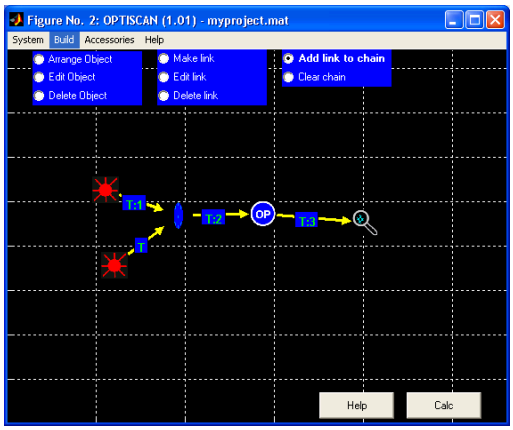


Figure 10

When setting up the optical element, the user must insure that the "vector" box is checked in the properties section, and that the propagation to target calculation is set on "map to curved exit pupil". By doing this the output of the optics calculation is the spectral components of the electric field incident on the grating, which is precisely the input to the RCWT mapping function.

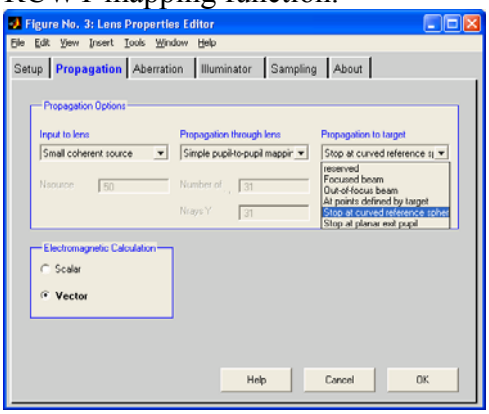


Figure 11

As was the case in the previous example, some time should be spent planning the RCWT calculation before beginning. In this case we are using 0.75 NA objective lens to focus a spot onto the grating structure. The grating structure has a sinusoidal profile with a period of 600nm and a wavelength of 633nm (these values are chosen to facilitate comparison with the values in reference 8 for the metal grating structure)

Because the input spectral sampling into the RCWT calculation is rather critical, extra care must be taken when defining the pupil sampling in the Optiscan LENS object. The value of Npupil set in the Lens Properties Editor is the number of discrete sample points across the *diameter* of the exit pupil. This number, divided by two should equal the numerical aperture of the imaging system divided by the pupil sampling used for the RCWT calculation. That is

$$Npupil/2 \approx NA/\Delta(n_1\alpha) = NA*d*PupS/\lambda.$$

It is not essential that this relationship be exactly satisfied, but care should be made to chose the pupil sampling as close as possible to the required value.

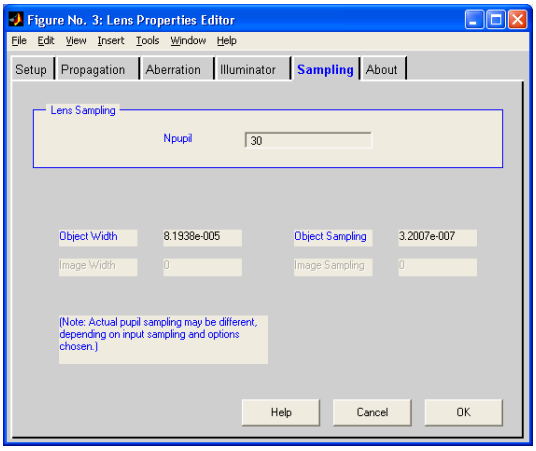


Figure 12

In practice, the user will generally chose the desired pupil sampling first (Npupil), then when calculating the RCWT basis set the value of PupS is chosen such that the above relationship is satisfied.

The source definition is not critical to the RCWT calculation, however, a small source is chosen small enough that the entrance pupil of the imaging system is fully illuminated.

The MOP script function used to map the data in the curved exit pupil of the optical system to the propagating wave fronts is as follows.

```
function [mop, curlink, simdata, errmsg] = mymop(action, mop, curlink, simdata)

    errmsg = '';

    Ex=simdata.Ext;
    Ey=simdata.Eyt;
    Ez=simdata.Ezt;

    xvec=simdata.sysxvec;
    yvec=simdata.sysyvec;
    lambda=simdata.LAMBDA;


    %get reference sphere radius
    lens=simdata.PrevObject;
    lens_data=load_lensfile(lens);
    PupData=pupil(1,lens_data);

    EXPZ=PupData.EXPZ/1000;

FILES.fnameZ=fullfile(mop,'<project>\<userdata>\','RCWT_SPZ');
```

```
FILES.fnameX=fullfile(mop,'<project>\<userdata>\','RCWT_SPX');
FILES.fnameY=fullfile(mop,'<project>\<userdata>\','RCWT_SPY');


%convert pupil coordiants into direction cosines
avecin=xvec/abs(EXPZ);
bvecin=yvec/abs(EXPZ);


%input data into RCWT
InPuP.PXin=sign(EXPZ)*Ex;
InPuP.PYin=sign(EXPZ)*Ey;
InPuP.PZin=Ez;

InPuP.avec=avecin;
InPuP.bvec=bvecin;

 [OutPup]=RCWTpupMAP(InPuP,FILES); %calculate the spectral mapping

PxR=OutPup.PxR;
PyR=OutPup.PyR;
PzR=OutPup.PzR;

PxT=OutPup.PxT;
PyT=OutPup.PyT;
PzT=OutPup.PzT;


avec=OutPup.avec;
bvec=OutPup.bvec;

    %update the source fields
    simdata.Exr = PxR;
    simdata.Eyr = PyR;
    simdata.Ezr = PzR;
simdata.sysxvec=avec;
simdata.sysyvec=bvec;

simdata.Ext = PxT;
simdata.Eyt = PyT;
simdata.Ezt = PxZ;
```

The first step in this script is to import the angular spectrum data from the lens object calculation. The spectrum arrays are stored in Ex, Ey and Ez, and the position vectors are stored in xvec and yvec. The position vectors in this case are physical dimensions in the exit pupil. The next step is to import some prescription data from the lens object.

specifically the distance between the image plane and the exit pupil (this value is stored in EXPZ). Dividing the physical position vectors in the exit pupil by the distance EXPZ gives the direction cosine vectors required for the RCWT calculation. Once these coordinates are calculated, the RCWT calculation is identical to the previous example, and the output is viewed using a LOOK object.

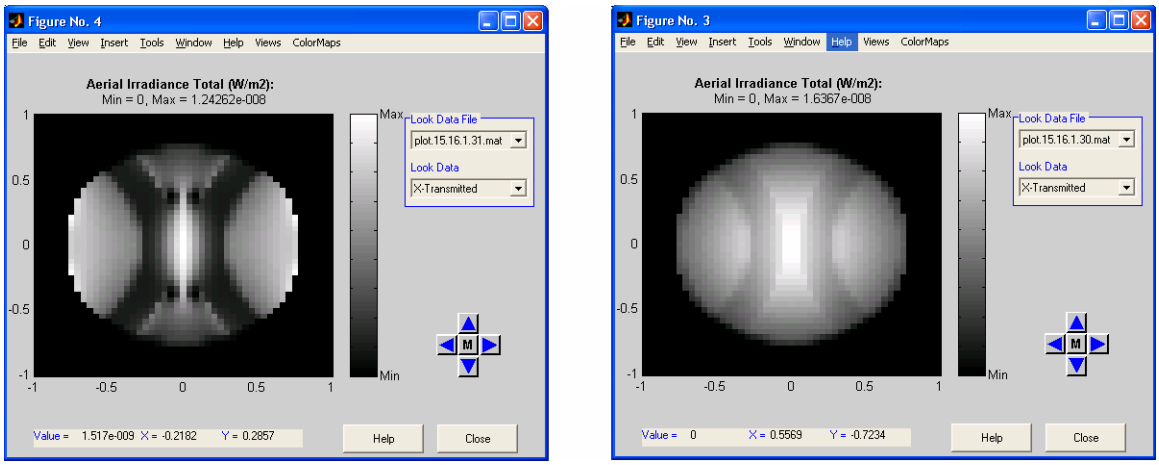


Figure 13

4.5 Mathematical Details

What follows is a detailed mathematical description of the RCWT basis set calculator in Optiscan.

The calculator begins by defining three angular spectrum functions of the form

$$A_x(\alpha_i,\beta_i) = cyl\left(\frac{\sqrt{(n_1\alpha_i)^2+(n_1\beta_i)^2}}{\text{NAmax}}\right)$$

$$A_y(\alpha_i,\beta_i) = cyl\left(\frac{\sqrt{(n_1\alpha_i)^2+(n_1\beta_i)^2}}{\text{NAmax}}\right) \qquad (4.1)$$

$$A_z(\alpha_i,\beta_i) = cyl\left(\frac{\sqrt{(n_1\alpha_i)^2+(n_1\beta_i)^2}}{\text{NAmax}}\right)$$

The sampling of each of these incident fields is $\Delta(n_1\alpha_i)=\lambda/(\text{PupS}*d)$ and $\Delta(n_1\beta_i)=\lambda/(\text{PupS}*d)$. These x,y and z angular spectra are converted into s and p spectra using the relationship

$$\begin{bmatrix} A_S(\alpha_i,\beta_i) \\ A_P(\alpha_i,\beta_i) \end{bmatrix} = \begin{bmatrix} \frac{-\beta_i}{\sqrt{\alpha_i^2+\beta_i^2}} & \frac{\alpha_i}{\sqrt{\alpha_i^2+\beta_i^2}} & 0 \\ \frac{\alpha_i\gamma_i}{\sqrt{\alpha_i^2+\beta_i^2}} & \frac{\beta_i\gamma_i}{\sqrt{\alpha_i^2+\beta_i^2}} & -\sqrt{\alpha_i^2+\beta_i^2} \end{bmatrix} \begin{bmatrix} A_x(\alpha_i,\beta_i) \\ A_y(\alpha_i,\beta_i) \\ A_z(\alpha_i,\beta_i) \end{bmatrix} \qquad (4.2)$$

However, for the RWCT calculator, the x,y and z spectra are transformed independently. For each incident s-polarized field $A_{xS}(\alpha_i,\beta_i)$ *corresponding to one of the incident states of polarization*, (that is, if the calculation is being performed for the x-polarized spectra

$A_{xS}(\alpha_i,\beta_i) = \frac{-\beta_i}{\sqrt{\alpha_i^2+\beta_i^2}}$) an RCWT calculation is performed with incident parameters

$$\begin{aligned} \theta_i &= \text{acos}(\gamma_i) \\ \phi_i &= \text{atan2}(\beta_i,\alpha_i) \\ \psi_i &= 90^o \end{aligned} \qquad (4.3)$$

where the atan2 operation removes the modulo π ambiguity of the atan operation. The result of this operation are four resultant spectra.

$$\begin{aligned} &R_{xSS}(\alpha,\beta;\alpha_i,\beta_i) \\ &R_{xSP}(\alpha,\beta;\alpha_i,\beta_i) \\ &T_{xSS}(\alpha,\beta;\alpha_i,\beta_i) \\ &T_{xSP}(\alpha,\beta;\alpha_i,\beta_i) \end{aligned} \qquad (4.4)$$

Likewise, for each incident s-polarized field $A_P(\alpha_i,\beta_i)$ an RCWT calculation is performed with incident parameters

$$\begin{aligned} \theta_i &= \text{acos}(\gamma_i) \\ \phi_i &= \text{atan2}(\beta_i,\alpha_i) \\ \psi_i &= 0^o \end{aligned} \qquad (4.5)$$

The result of this operation are four resultant spectra.

$$\begin{aligned} &R_{xPS}(\alpha,\beta;\alpha_i,\beta_i) \\ &R_{xPP}(\alpha,\beta;\alpha_i,\beta_i) \\ &T_{xPS}(\alpha,\beta;\alpha_i,\beta_i) \\ &T_{xPP}(\alpha,\beta;\alpha_i,\beta_i) \end{aligned} \qquad (4.6)$$

The reflected polarization spectra for the incident electric field is given by

$$\begin{aligned} R_{xS}(\alpha,\beta;\alpha_i,\beta_i) &= R_{xSS}(\alpha,\beta;\alpha_i,\beta_i) + R_{xPS}(\alpha,\beta;\alpha_i,\beta_i) \\ R_{xP}(\alpha,\beta;\alpha_i,\beta_i) &= R_{xSP}(\alpha,\beta;\alpha_i,\beta_i) + R_{xPP}(\alpha,\beta;\alpha_i,\beta_i) \\ T_{xS}(\alpha,\beta;\alpha_i,\beta_i) &= T_{xSS}(\alpha,\beta;\alpha_i,\beta_i) + T_{xPS}(\alpha,\beta;\alpha_i,\beta_i) \\ T_{xP}(\alpha,\beta;\alpha_i,\beta_i) &= T_{xSP}(\alpha,\beta;\alpha_i,\beta_i) + T_{xPP}(\alpha,\beta;\alpha_i,\beta_i) \end{aligned} \qquad (4.7)$$

Therefore, a unit amplitude x-polarized plane wave propagating with direction cosines α_i and α_i is mapped into these four resultant spectra. These fields are then saved by the RCWT basis set generator, along with the incident coordinate position α_i and β_i, as well as other assorted data associated with the calculation. Note that the sampling of each resultant spectra is given by $\Delta\alpha=\Delta\beta=\lambda/d$ (this output sampling is a result of the RCWT algorithm).

Converting an arbitrary incident field whose spectra is given by $\left\{A'_x(\alpha_i,\beta_i), A'_y(\alpha_i,\beta_i), A'_z(\alpha_i,\beta_i)\right\}$ (where it is assumed that the incident spectra have been interpolated into grid with angular sampling given by $\Delta(n_1\alpha_i)=\lambda/(PupS*d)$ and $\Delta(n_1\beta_i)=\lambda/(PupS*d)$), one simply multiplies the incident spectra by the precalculated basis set. That is, for the incident x-polarization

$$\begin{aligned} R'_{xS}(\alpha,\beta;\alpha_i,\beta_i) &= A'_x(\alpha_i,\beta_i)\,R_{xS}(\alpha,\beta;\alpha_i,\beta_i) \\ R'_{xP}(\alpha,\beta;\alpha_i,\beta_i) &= A'_x(\alpha_i,\beta_i)\,R_{xP}(\alpha,\beta;\alpha_i,\beta_i) \end{aligned}. \qquad (4.8)$$

Therefore, the S and P reflected spectra resulting from the incident x-polarized spectra are mapped onto the output array in a point by point fashion. This results in arrays representing the S and P components of the reflected and transmitted electric fields. These arrays are converted to X, Y and X components using the inverse of the mapping given in Eq.(4.2)

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