# Thin Film Calculator Manual

In this report, thin film model is explained. The background of thin film model is explained at the beginning, and followed with the theory for calculating the amplitude reflection/transmission coefficients, phase change, as well as reflectance and transmittance. MATLAB codes are given then based on the theory, and it is used to design a broadband reflector for the visible region of design. The results are compared with the published data in Professor Angus Macleod's class notes. [1] Finally, the MATLAB codes are included in OptiScan for a user friendly interface. An example in Thin Film Calculator in OptiScan is given to calculator the reflectance and transmittance of Krestchmann configuration which generate surface plasma resonance at a certain incident angle.

## 1.  Background [1]

Optical systems consist of a series of boundaries between different materials. These surfaces are usually optically worked so that their properties are specular, that is the directions of light obey the laws of reflection and refraction, and their shape is adjusted to a desired manner, such as minimizing the aberrations. Unfortunately the other properties of the surfaces, such as reflectance, transmittance, or phase change, are rarely satisfied. Thin films are commonly used to modify these properties without altering the specular behavior.

In an optical coating, the films, together with their support, or substrate, are generally solid. The particular materials used for the films vary with the applications. It is possible to construct assemblies of thin films which will reduce the reflectance of a surface and hence increase the transmittance of a component, or increase the reflectance of a surface, or which will give high reflectance and low transmittance over part of a region and low reflectance and high transmittance over the remainder and so on. Thin film coatings are often known by names which describe their function, such as antireflection coatings, beam splitters, polarizers, long-wave-pass filters, band-stop or minus filters, or which describe their construction, such as quarter-wave stack, quarter-half-quarter coating and so on.

In a thin-film assembly, the amount of light reflected at each interface depends on the refractive indices of the materials on either side and thus the magnitudes of the various beams involved in the interference can be adjusted by choosing the refractive indices of the films. The phases of the beams on the other hand can be adjusted by changing the layer thickness. There are thus two parameters associated with each layer, thickness and refractive index, which can be chosen to give the required performance. Complete freedom of choice is not possible since suitable coating materials are limited, then the optimum theoretical performance will be also limited. Additionally there will be inevitable drops in performance manufacture due to constructional variations.

A film in an optical coating is said to be thin when interference effects can be detected in the light which it reflects or transmits, and thick when they cannot. Of course, whether or not interference effects can be detected, depends as much on the source of illumination and the receiver which is used, as on the films themselves. Even without

changing the wavelength, the same film can be made to appear thick or thin, depending entirely on illumination and detection conditions. In normal coating, the films will be thin while the substrates will be thick.

Thin film calculator is a program which is embedded in OptiScan which can be used to calculate the amplitude reflection and transmission coefficients, phase change, reflectance and transmittance of both s and p polarized light. The theory is briefly explained in the following section, which is based on matching the boundary conditions for Maxwell's equations. Interested readers can find the detailed information in Prof. Angus Macleod's notes "Optical Thin Films". [1]

## 2. Theory of Thin Film Model [1]

In thin film model, only linear, isotropic and homogeneous films are considered. In these medium, the electric and magnetic fields of a harmonic wave are connected through another material parameter, the characteristic admittance, y.

$$H = yE$$

The characteristic admittance varies with wavelength but in free space it is constant. The optical admittance of free space as $\eta_{free}$ is given by

$$\eta_{free} = \sqrt{\frac{\varepsilon_0}{\mu_0}} = 2.6544 \times 10^{-3} S$$

For an arbitrary medium at given wavelength, the characteristic admittance, y, can be written as the following.

$$y = (n - ik)\eta_{free}$$

This relationship is good through the whole of the optical region, which means for all wavelengths shorter than several hundred microns. $(n - ik)$ is the complex refractive index for the medium. Please be carefully for the sign and convention here, since normally $(n + ik)$ is used as the complex refractive of medium. But in thin film community, $(n - ik)$ is used. In the MATLAB codes, $(n - ik)$ is used as the format to input refractive index of films. However in OptiScan, $(n + ik)$ is used as the input refractive index of films in order to be consistent with the definitions in OptiScan.
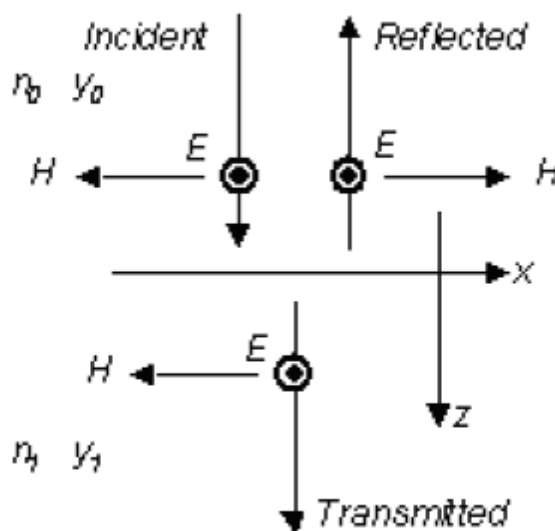
Fig 2-1. Normal incidence at a surface and the sign convention for fields [1]

Amplitude reflection coefficient, $\rho$, that is the ratio of the reflected amplitude to the incident amplitude, and the amplitude transmission coefficient, $\tau$, that is the ratio of

the transmitted amplitude to the incident amplitude. In a normal incidence of thin film structure, as shown in Fig 2-1, by matching the boundary conditions for Maxwell's equations, their expressions can be calculated in thin film model with the results given as:

$$\rho = \frac{\eta_0 - Y}{\eta_0 + Y}$$

$$\tau = \frac{2\eta_0}{\eta_0 + Y}$$

where, $\eta_0$ is the surface admittance for incident medium, and $Y$ is the surface admittance of the thin films and substrate, which can be calculated from the following equations.

$$Y = \frac{C}{B}$$

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{ \prod_{j=1}^{q} \begin{bmatrix} cos\delta_j & \dfrac{isin\delta_j}{y_j} \\ iy_j sin\delta_j & cos\delta_j \end{bmatrix} \right\} \begin{bmatrix} 1 \\ y_{sub} \end{bmatrix}$$

where,

$B$ and $C$ are normalized total tangential electric and magnetic fields respectively at the input surface

$\delta_j = \frac{2\pi(n_j - ik_j)d_j}{\lambda}$ is the phase thickness of layer j

$(n_j - ik_j), d_j$ are the complex index and physical thickness of layer j

$y_j$ is the characteristic admittance of layer j

$q$ is the number of layers and layer $q$ is next to the substrate

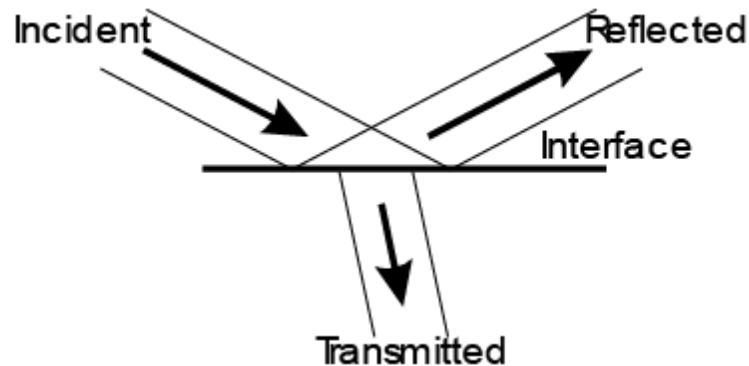$y_{sub}$ is the characteristic admittance of the substrate



Fig 2-2. Refraction tilts the transmitted beam with respect to the incident beam and so, although both beams are drawn with the same cross sectional area, they subtend different areas at the boundary. [1]

Reflectance, $R$, as the ratio of the irradiance of the reflected beam to that of the incident beam, and transmittance, $T$, as the ratio of the irradiance of the transmitted beam to that of the incident beam, as shown in Fig 2-2, are defined as:

$$R = \rho\rho^* = \left[\frac{\eta_0 - Y}{\eta_0 + Y}\right]\left[\frac{\eta_0 - Y}{\eta_0 + Y}\right]^*$$

$$T = \frac{4\eta_0 Re(Y)}{(\eta_0 + Y)(\eta_0 + Y)^*}$$

As we can see from above, the effects of multiple films are included in the surface admittance $Y$. Each layer generates a matrix in the equation which will change the electric and magnetic fields. The finally results are only related to the admittance of incident medium and the surface admittance of the thin films and substrate. Since the

reflectance cannot be defined in an absorbing incident medium, $y_0$ has to be real. The units of admittance are cancelled in the calculation.

The equations given above are suitable for normal incidences. However, in general, oblique incidence is more commonly used. At oblique incidence, there are two states where the components remain in the same plane, one with electric vector parallel to the plane of incidence, knows as *p*-polaried light, and one with electric vector perpendicular to the plane of incidence, knows as *s*-polaried light. Only in these two cases the polarization states of the incident beam will be preserved in the reflected and transmitted beams, as shown in Fig 2-3. Any arbitrary polarizations can be split into a combination of these two components which can be solved separately, and the final result then given by the combination of the two solutions.
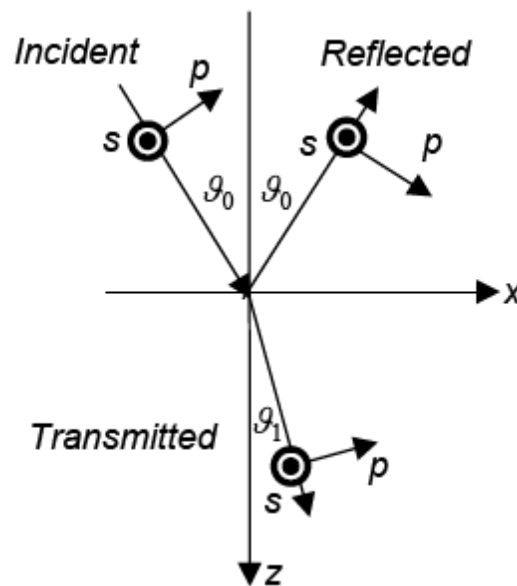


Fig 2-3. *p*-polarized and *s*-polarized light for oblique incidence. [1]

In thin film model, the tangential components are used to define the reflection and transmission coefficient. This is different from the Fresnel coefficients, which uses the total electric and magnetic fields of the waves. However, the differences are confined to the amplitude transmission coefficient for $p$-polarized light.

$$\rho = \frac{reflected\ amplitude\ (tangential\ component)}{incident\ amplitude\ (tangential\ component)}$$

$$\tau = \frac{transmitted\ amplitude\ (tangential\ compnent)}{incident\ amplitude\ (tangential\ component)}$$

The definitions for surface optical admittance retains as the ratio of the components of magnetic and electric fields parallel to the interfaces but since this is different for the two modes of polarization we need two calculations. The expressions for amplitude reflection/transmission coefficients, reflectance and transmittance are still valid if we replace the admittance with the tiled admittance for $s$-polarized and $p$-polarized light.

$s$-polarization:

$$Optical\ admittance = \eta_s = ycos\theta = (n-ik)cos\theta$$

$p$-polarization:

$$Optical\ admittance = \eta_s = y/cos\theta = (n-ik)/cos\theta$$

Once again we emphasize that the amplitude reflection and transmittance components are not strictly the Fresnel components. In fact, all except $\tau_p$ do coincide with the Fresnel expressions.

# 3. MATLAB codes and examples

In this section, the MATLAB code of thin film calculator is given, as well as an example of the broadband reflector design for the visible region. Two functions *multilayer_s.m* and *multilayer_p.m* are built in MATLAB for different polarization incident light, and they are the core program of thin film calculator. They calculate the amplitude reflection/transmission coefficients, reflectance and transmittance.

The way to use these programs is shown below:

For *s*-polarized light:

```
function [rho,tao,R,T] = multilayer_s(d,y,y_inc,y_sub,lambda,theta);
```

For *p*-polarized light:

```
function [rho,tao,R,T] = multilayer_p(d,y,y_inc,y_sub,lambda,theta);
```

For arguments, *multilayer_s.m* and *multilayer_p.m* require:

      d: thin film thickness (thickness for the film next to incident medium is first)

      y: admittance or refractive index in the form of $(n - ik)$ (admittance for the film

         next to the incident medium is first)

      y_inc: admittance of incident medium in the form of $(n - ik)$

      y_sub: admittance of substrate in the form of $(n - ik)$

      lambda: wavelength of incident light

      theta: incident angle (unit in degree, can be a vector)

The outputs are:

rho: the complex reflection coefficient (including amplitude reflection coefficient

and phase change)

tao: the complex transmission coefficient (including amplitude transmission

coefficient   and phase change)

R: reflectance

T: transmittance

One example is provided in MATLAB code to show how to use *multilayer_s.m* in the following, which is a broadband reflector for the visible region. Twenty three films are coated on glass substrate. The reference wavelength is 480nm, two types of materials are used for the coating with indices: 2.35 (H), and 1.35 (L). The geometry is given in the table in the following. The thickness is given in the units of reference wavelength. And optical thickness is used in the table instead of physical thickness for a better understanding of the phase change of each film. The optical thickness differs from physics thickness by a factor of index.

Optical thickness is defined as:

$$\text{optical thickness} = \text{index} \times \text{physical thickness}$$

The reflectance calculated from *multilayer_s.m* is given in Fig 3-1, which is compared with the published result in Macleod's "Optical thin films", which is given in Fig 3-2.

Table 1: Broadband Reflector for Visible Region Design [1]

| Layer | Index | Thickness | Layer | Index | Thickness |
|---|---|---|---|---|---|
| 0 | 1 | Incident | 13 | 2.35 | 1.4*0.25 |
| 1 | 2.35 | 0.25 | 14 | 1.35 | 1.4*0.25 |
| 2 | 1.35 | 0.25 | 15 | 2.35 | 1.4*0.25 |
| 3 | 2.35 | 0.25 | 16 | 1.35 | 1.4*0.25 |
| 4 | 1.35 | 0.25 | 17 | 2.35 | 1.4*0.25 |
| 5 | 2.35 | 0.25 | 18 | 1.35 | 1.4*0.25 |
| 6 | 1.35 | 0.25 | 19 | 2.35 | 1.4*0.25 |
| 7 | 2.35 | 0.25 | 20 | 1.35 | 1.4*0.25 |
| 8 | 1.35 | 0.25 | 21 | 2.35 | 1.4*0.25 |
| 9 | 2.35 | 0.25 | 22 | 1.35 | 1.4*0.25 |
| 10 | 1.35 | 0.25 | 23 | 2.35 | 1.4*0.25 |
| 11 | 2.35 | 0.25 | 24 | 1.52 | Substrate |
| 12 | 1.35 | 1.2*0.25 | | | |

Note: reference wavelength $\lambda_f = 480nm$, and the thickness above is optical thickness instead of physical thickness, with the unit of reference wavelength. Optical thickness is defined as:

$$\text{optical thickness} = \text{index} \times \text{physical thickness}$$

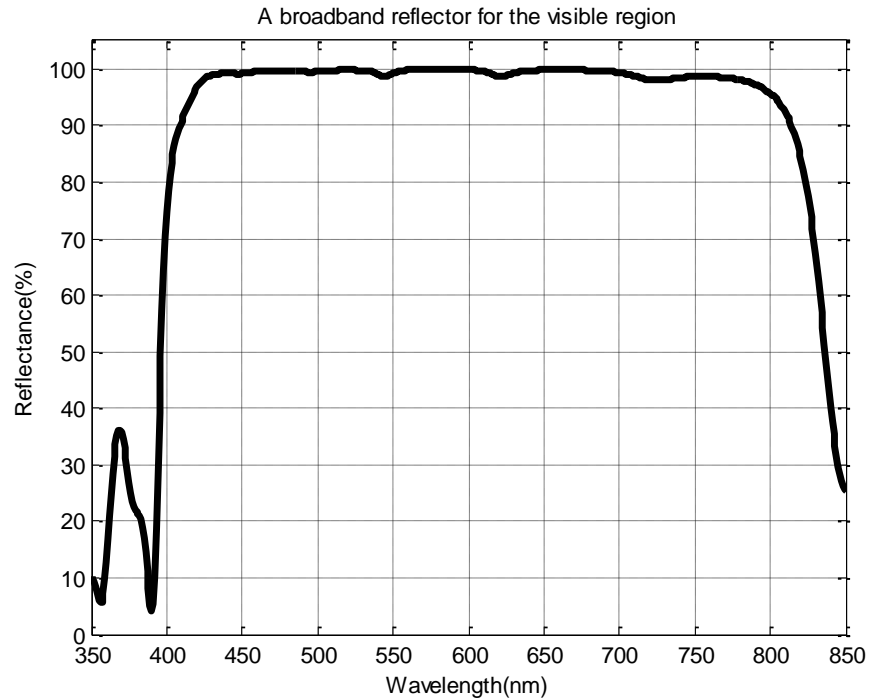A broadband reflector for the visible region

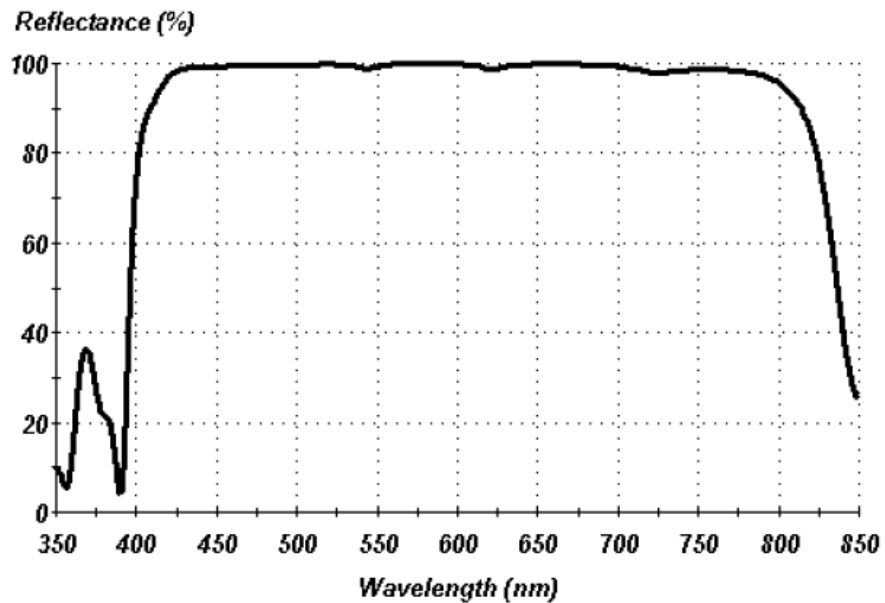Fig 3-1 Reflectance for broadband reflector from thin film calculator

Figure 4-27. A broadband reflector for the visible region of design:
Air | $(HL)^5$ H 1.2$L$ (1.4$H$ 1.4$L)^5$ 1.4H | Glass with $y_H$=2.35, $y_L$=1.35 and $y_{glass}$=1.52. The reference wavelength is 480nm.

Fig 3-2 Reflectance for broadband reflector from Macleod's notes [1]

### 3.1 thin_film_cal_example.m

```matlab
% This program is an example to use thin film model. The design if a
% broadband reflector for the visible region of design.
% Data resource: Figure 4-27 in "Optical thin film"

% initial program

clear all;
close all;


um      = 1e-6;
nm      = 1e-9;

% define admittance for medium
Air     = 1;
yH      = 2.35;
yL      = 1.35;
Glass   = 1.52;

% define the reference wavelength and thickness
lambda_f    = 480*nm;
dH      = lambda_f/4/yH; % quarter stack
dL      = lambda_f/4/yL;

% define visible region of light
lambda  = linspace(350,850,501)*nm;

% define thin film structure
y_inc   = Air; % incident medium admittance
y_sub   = Glass; % substrate medium admittance
theta   = 0; % in degree
d       =
[dH,dL,dH,dL,dH,dL,dH,dL,dH,dL,dH,1.2*dL,1.4*dH,1.4*dL,1.4*dH,1.4*dL,...
        1.4*dH,1.4*dL,1.4*dH,1.4*dL,1.4*dH,1.4*dL,1.4*dH];
y       = [yH,yL,yH,yL,yH,yL,yH,yL,yH,yL,yH,yL,yH,yL,yH,yL,...
        yH,yL,yH,yL,yH,yL,yH];

for ii=1:length(lambda),
    [rho(ii),tao(ii),R(ii),T(ii)]   =
multilayer_s(d,y,y_inc,y_sub,lambda(ii),theta);
end

% plot the result
figure, plot(lambda/nm,R*100,'-k','LineWidth',3);
title('A broadband reflector for the visible region');
xlabel('Wavelength(nm)');
ylabel('Reflectance(%)');
axis([350 850 0 105]);
grid on;
```

### 3.2 multilayer_p.m

```matlab
function [rho,tao,R,T] = multilayer_p(d,y,y_inc,y_sub,lambda,theta)

% This code is for p-polarization.

for m = 1:length(theta),
    for i = 1:length(y),
        y_s(m,i)        = sqrt(real(y(i))^2-imag(-y(i))^2-
y_inc^2*sind(theta(m))^2-2*1i*real(y(i))*imag(-y(i)));
        if imag(y_s(m,i))>0,
            y_s(m,i)    = -(y_s(m,i));
        end
        delta_s(m,i)    = 2*pi*d(i)/lambda*y_s(m,i);
        y_inc_s(m)      = y_inc*cosd(theta(m));
        y_sub_s(m)      = sqrt(real(y_sub)^2-imag(-y_sub)^2-
y_inc^2*sind(theta(m))^2-2*1i*real(y_sub)*imag(-y_sub));
        if imag(y_sub_s(m))>0,
            y_sub_s(m)  = -(y_sub_s(m));
        end
        y_p(m,i)        = y(i)^2/y_s(m,i);
        delta_p(m,i)    = delta_s(m,i);
        y_inc_p(m)      = y_inc^2/y_inc_s(m);
        y_sub_p(m)      = y_sub^2/y_sub_s(m);
        tmp     = [cos(delta_p(m,i)),  1i*sin(delta_p(m,i))/y_p(m,i);
                   1i*y_p(m,i)*sin(delta_p(m,i)),  cos(delta_p(m,i))];
        if i == 1,
            M   = tmp;
        else
            M   = M*tmp;
        end
    end
    BC      = M*[1; y_sub_p(m)];
    B(m)    = BC(1);
    C(m)    = BC(2);

% rho and tao are the amplitude reflection and transmission
% coefficients
    rho(m)      = (y_inc_p(m)*B(m)-C(m))/(y_inc_p(m)*B(m)+C(m));
    phi_r(m)    = angle(rho(m))/pi*180; % phase
    tao(m)      = 2*y_inc_s(m)/(y_inc_s(m)*B(m)+C(m));
    phi_t(m)    = angle(tao(m))/pi*180; % phase

% R and T are the intensity reflection and transmission coefficients
% Note: for transmission, the angle changes due to refraction, thus
area is
% different

    R(m)    = abs(rho(m))^2;
    T(m)    =
4*y_inc_p(m)*real(y_sub_p(m))/abs((y_inc_p(m)*B(m)+C(m)))^2;
end
```

### 3.3 multilayer_s.m

```
function [rho,tao,R,T] = multilayer_s(d,y,y_inc,y_sub,lambda,theta)

% This code is for s-polarization.

for m = 1:length(theta),
    for i = 1:length(y),
        y_s(m,i)         = sqrt(real(y(i))^2-imag(-y(i))^2-
y_inc^2*sind(theta(m))^2-2*1i*real(y(i))*imag(-y(i)));
        if imag(y_s(m,i))>0,
            y_s(m,i)     = -(y_s(m,i));
        end
        delta_s(m,i)     = 2*pi*d(i)/lambda*y_s(m,i);
        y_inc_s(m)       = y_inc*cosd(theta(m));
        y_sub_s(m)       = sqrt(real(y_sub)^2-imag(-y_sub)^2-
y_inc^2*sind(theta(m))^2-2*1i*real(y_sub)*imag(-y_sub));
        if imag(y_sub_s(m))>0,
            y_sub_s(m)   = -(y_sub_s(m));
        end
        tmp     = [cos(delta_s(m,i)),  1i*sin(delta_s(m,i))/y_s(m,i);
                    1i*y_s(m,i)*sin(delta_s(m,i)), cos(delta_s(m,i))];
        if i == 1,
            M   = tmp;
        else
            M   = M*tmp;
        end
    end
    BC      = M*[1; y_sub_s(m)];
    B(m)    = BC(1);
    C(m)    = BC(2);

% rho and tao are the amplitude reflection and transmission
coefficients
    rho(m)    = (y_inc_s(m)*B(m)-C(m))/(y_inc_s(m)*B(m)+C(m));
    phi_r(m)  = angle(rho(m))/pi*180; % phase
    tao(m)    = 2*y_inc_s(m)/(y_inc_s(m)*B(m)+C(m));
    phi_t(m)  = angle(tao(m))/pi*180; % phase

% R and T are the intensity reflection and transmission coefficients
% Note: for transmission, the angle changes due to refraction, thus
area is
% different
    R(m)    = abs(rho(m))^2;
    T(m)    =
4*y_inc_s(m)*real(y_sub_s(m))/abs((y_inc_s(m)*B(m)+C(m)))^2;
end
```

# 4. Thin Film Calculator in OptiScan

One example is provided in the following to show how to use Thin Film Calculator to calculate the amplitude reflection, transmission coefficients, phase change, reflectance and transmittance for s and p polarized light in OptiScan. The geometry is described in the following table. A high index glass (S-LAH79) is used as the incident medium. 45nm silver is coated on the glass to generate the surface plasma resonance, and 30nm SiO2 layer is used to protect silver from oxidation. Tested sample is located next to SiO2 layer, and is the substrate of the geometry. The wavelength is 632.8nm.

Table 4.1: Example geometry

|  | Material | Index | Thickness (nm) |
|---|---|---|---|
| Incident medium | S-LAH79 | 1.99613 | -- |
| Metal coating | Silver | 0.135+3.987i | 45 |
| Protective coating | SiO2 | 1.45708 | 30 |
| Substrate | Water | 1.33258 | -- |

The following are the procedures to simulate this structure in Thin Film Calculator in OptiScan. [2]

1. First, OptiScan needs to be started. Choose the correct directory for OptiScan, and type "startup" in the command window, the opening panel looks like that in Fig 4-1.



Fig 4-1: starting panel for OptiScan

2. Open a new project in OptiScan, save the project, and then a window for the main project is opened and looks like Fig 4-2.
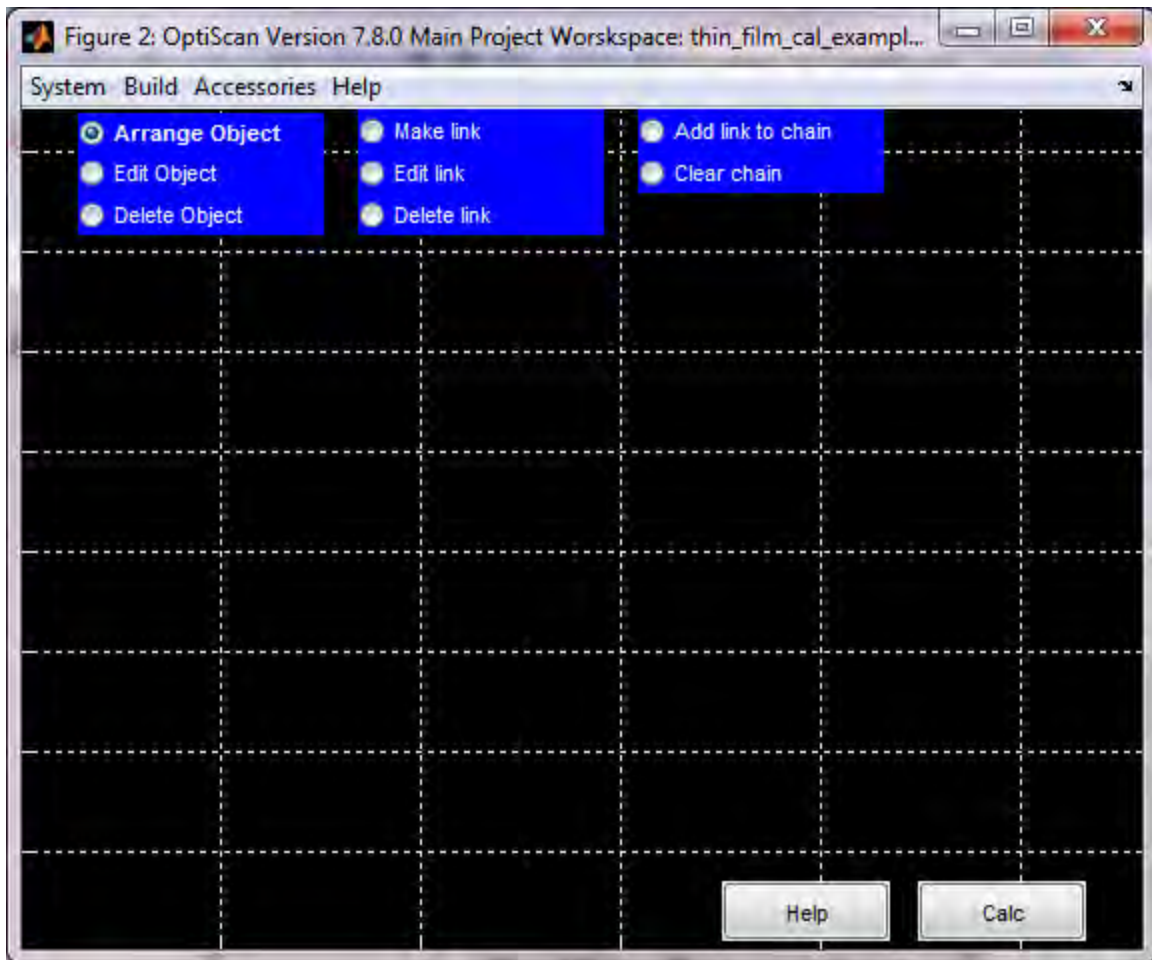
Fig 4-2: Main project window

3. Click on the "Accessories" on the main project window, and then choose the "Thin Film Calculator". A new window for "Thin Film Calculator" looks like that in Fig 4-3. The first four parameters refer to the "Index of Incident Medium", "Index of Substrate", "Wavelength", and "From angle". In our example, use 1.99613 for index of incident medium, 1.54265 for index of substrate, 632.8e-9 for wavelength (unit in meter), and 0 to 90 for angle (unit in degree).
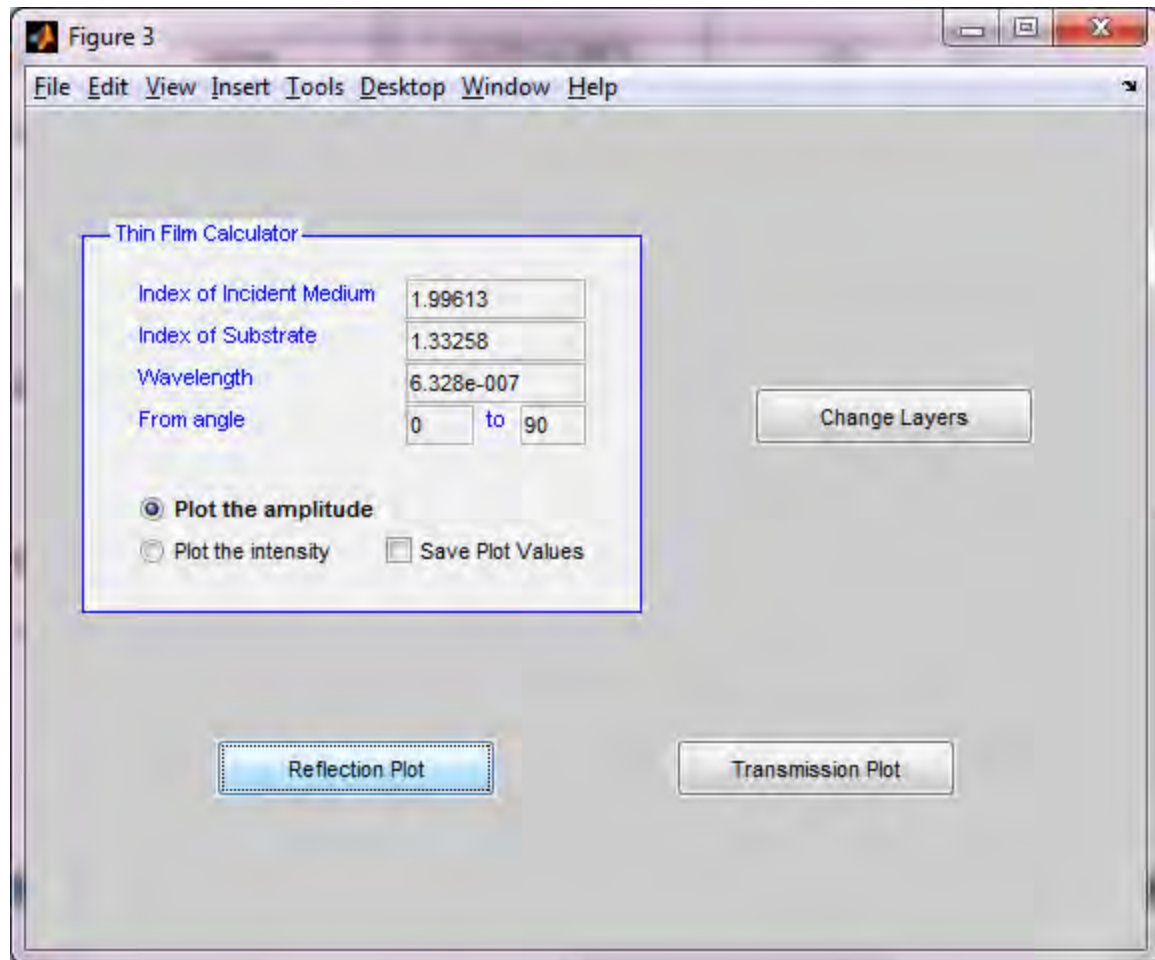
Fig 4-3: Thin Film Calculator panel window

4. Input the thin film layers, press the "Change Layers" to modify the "TFT Layers". Multiple thin film layers can be added in OptiScan, and this can be done by clicking "New Layer" in the "Tools" in this panel. The order of the layers is defined as the following: the first layer is the one next to the incident medium, and the last layer is the one on top of substrate. In case that there is no layer between the incident and substrate mediums, it is suggested that a very thin film with the same material as the incident or substrate medium can be used for "TFT Layers". It is suggested that empty TFT layers is

not used. The panel for "TFT Layers" is given in Fig 4. For each layer, two layer parameters are needed: refractive index and thickness. Click on "TFT Layer" on Layer list to select the layer (in blue). Then input the two parameters in "N" and "Thick" in "Layer Parameters". The unit for thickness is meters. Repeat these procedures for other layers. Use "Cut" button to delete the unwanted layers. After all the parameters have been assigned for TFT layers, click "OK" to return back to the Thin Film Calculator panel. Fig 4 and Fig 5 are the windows for different layers. Fig 4-4 is the silver coating, and Fig 4-5 is the SiO2 layer.
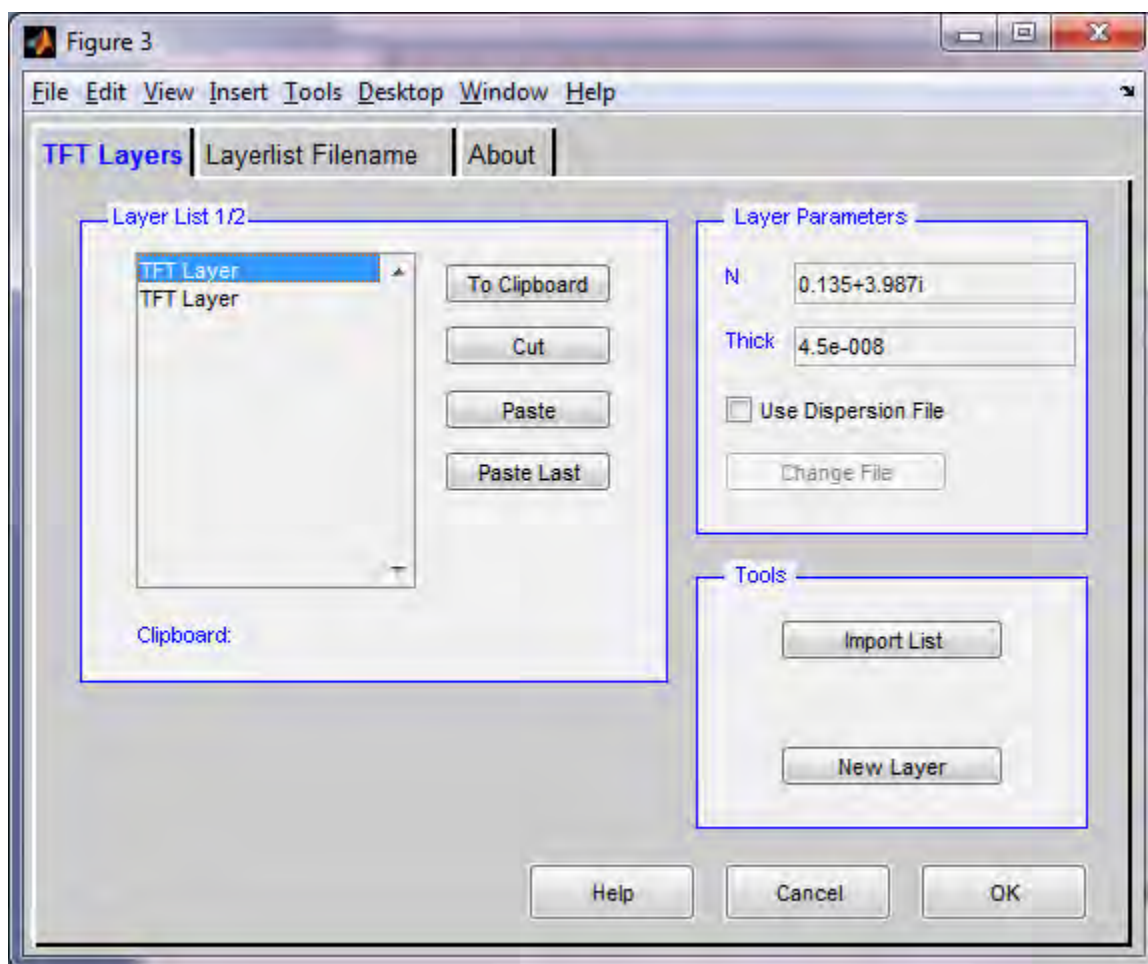


Fig 4-4. TFT Layers window for silver film with index 0.135+3.987i, and thickness 45nm.
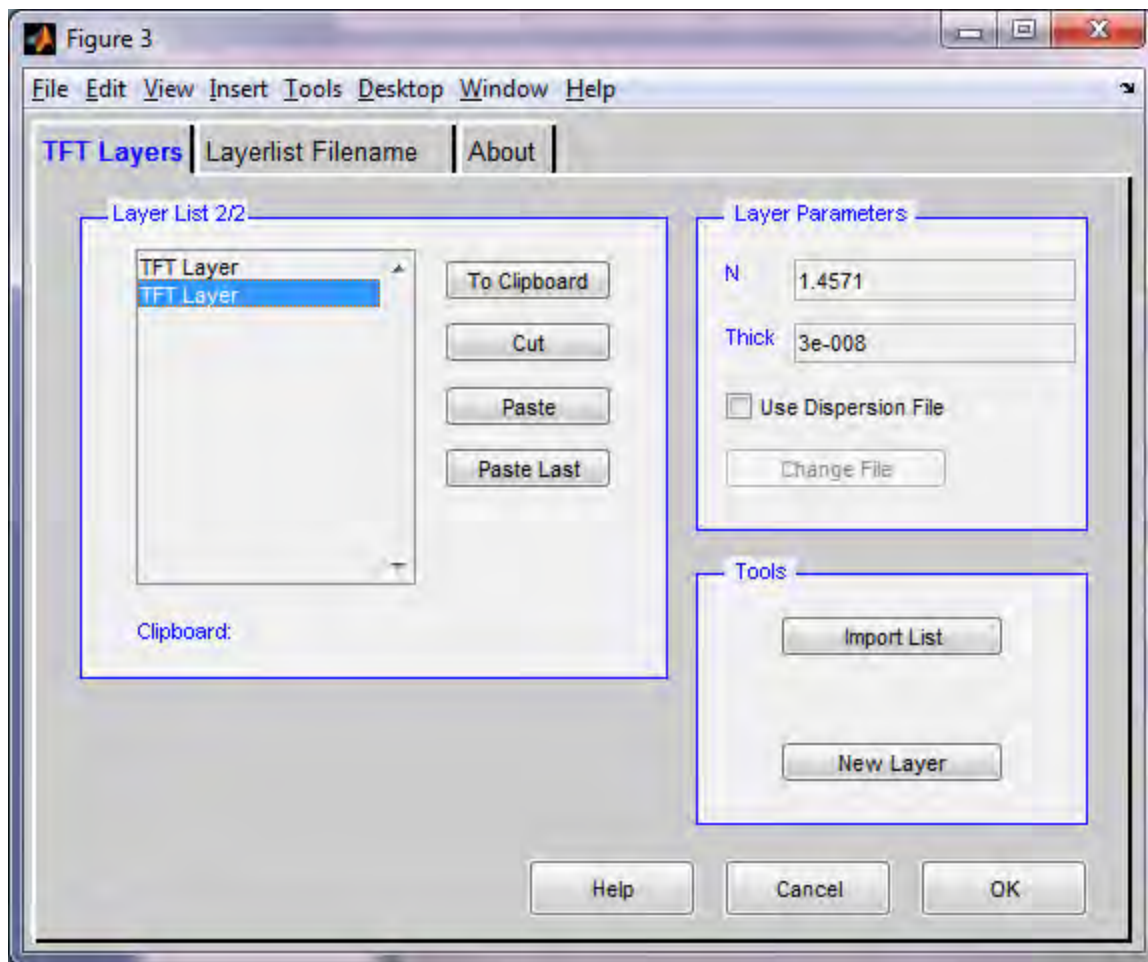
Fig 4-5. TFT Layers window for SiO2 film with index 1.4571, and thickness 30nm.

5. Calculate the amplitude reflection and transmission coefficients, and phase change. In the Thin Film Calculator panel, select "Plot the amplitude", and then click the "Reflection Plot" button for plotting the amplitude reflection coefficients for s and p polarized light. The phase change for s and p polarized light are also given in the results window, as shown in Fig 4-6. Return back to the Thin Film Calculator panel, and click "Transmission Plot" to plot the amplitude transmission coefficients and phase change for s and p polarized light. The results window is given in Fig 4-7.
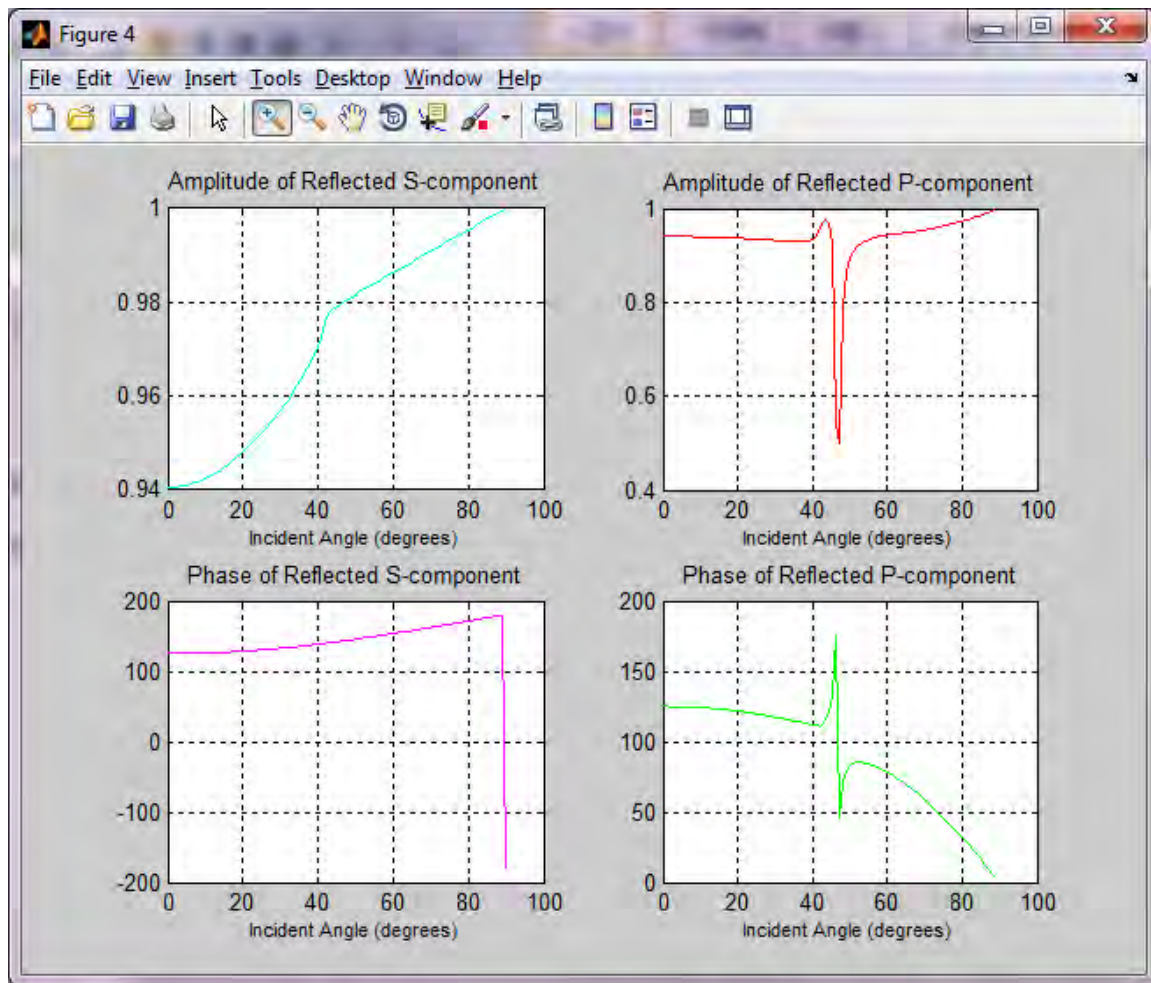
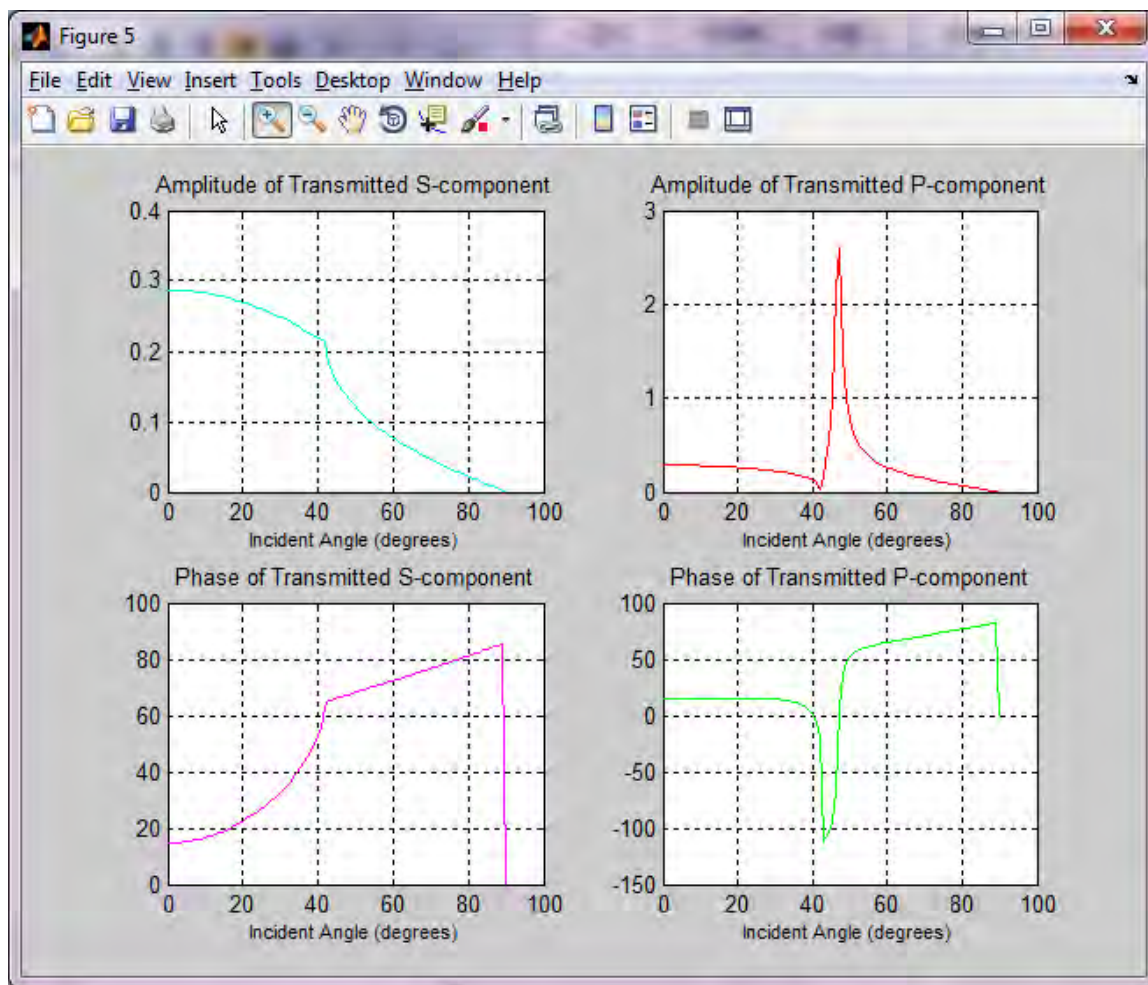Fig 4-6. Amplitude reflection coefficients and phase change for s and p polarized light.

Fig 4-7. Amplitude transmission coefficients and phase change for s and p polarized light.

6. Calculator the reflectance and transmittance for the geometry. Return back to the Thin Film Calculator panel, and click "Plot the intensity". Click on the "Reflection Plot" for the reflectance curves for s and p polarized light. Note that phase change is set to zero now since only intensity is considered. The result for reflectance is given in Fig 4-8. Similarly, click on "Transmission Plot" for the transmittance curves for s and p polarized light. The result for transmittance is given in Fig 4-9.
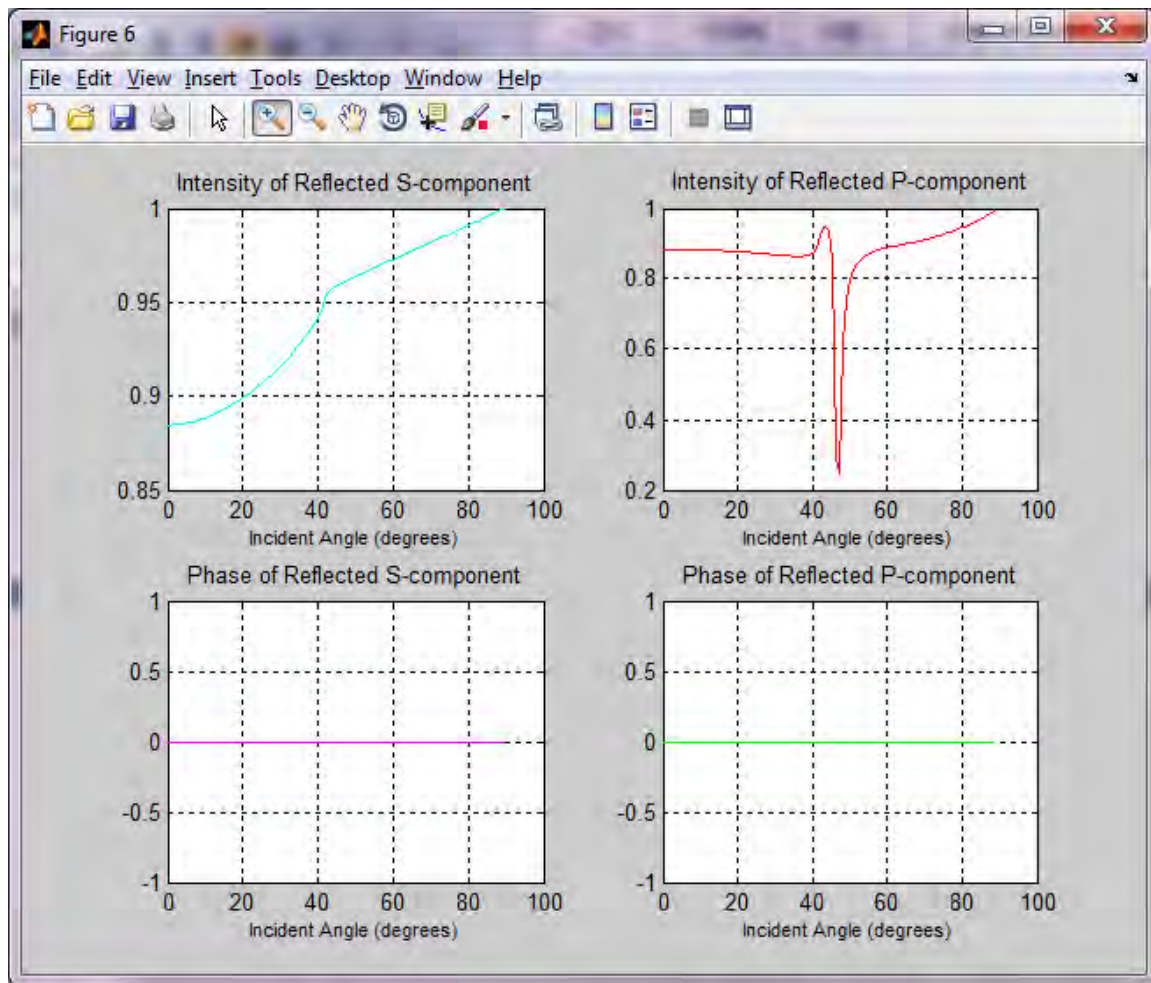
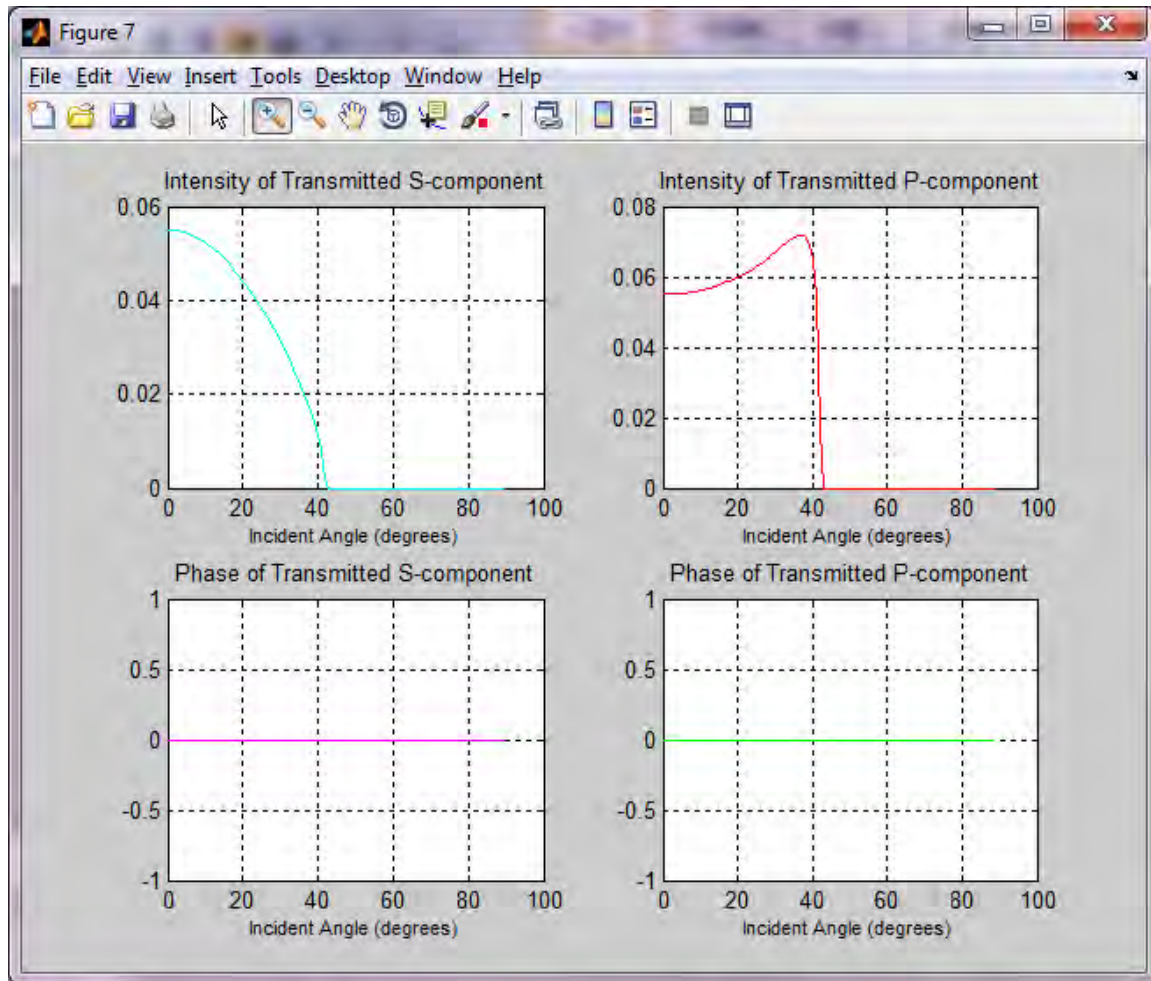Fig 4-8. Reflectance for s and p polarized light.

Fig 4-9. Transmittance for s and p polarized light.

7.  Save the results. In Thin Film Calculator panel, click on "Save Plot Values". Then when clicking on "Reflection Plot" or "Transmission Plot", a window is given as Fig 4-10 to ask a directory and name for the saved files. Choose the directory to save the file and type the file name. Then click on "Save", results window will be given and also be saved.
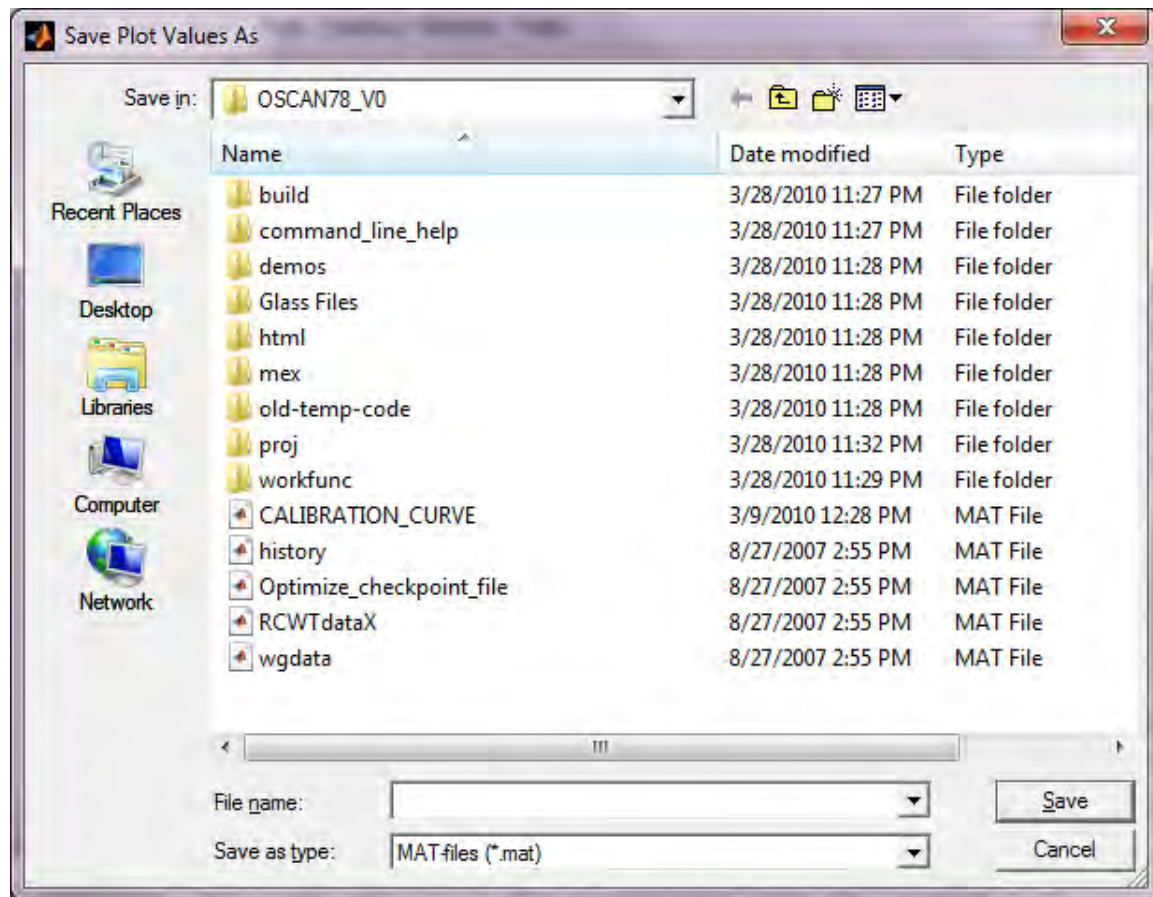
Fig 4-10. Save plot values panel.

# 5. References

[1]  H Augus Macleod, class notes for Opti575,  "Optical Thin Films"

[2]  OptiScan Manual