DEVELOPMENT OF SOFTWARE FOR CALCULATIONS OF THE REFLECTANCE, TRANSMITTANCE AND ABSORPTANCE OF MULTILAYERED THIN FILMS

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ABSTRACT

DEVELOPMENT OF SOFTWARE FOR CALCULATIONS OF THE REFLECTANCE, TRANSMITTANCE AND ABSORPTANCE OF MULTILAYERED THIN FILMS

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The aim of this study is to develop a software which calculates reflection, transmission and absorption of multilayered thin films by using complex indices of refraction, as a function of both wavelength and thickness. For these calculations matrix methods will be considered and this software is programmed with the matrix method. Outputs of the program will be compared with the theoretical and experimental results studied in the scientific papers.

Keywords: thin films, multilayer coating, optical films, software, programming.

ÖZ

ÇOK KATMANLI İNCE FİLMLERİN YANSIMA, GEÇİRME VE SOĞURMA ORANLARINI HESAPLAMADA KULLANILACAK YAZILIMIN GELİŞTİRİLMESİ

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Bu çalışmanın amacı, çok katmanlı ince filmler için kırılma indisinin kompleks kısmını da kullanarak yansıma, geçiş ve emilimi, dalgaboyu ve kalınlığın birer fonksiyonu olarak hesaplayan yazılımın geliştirilmesidir. Bu hesaplamalar için matris metodu ele alınacaktır. Bu yazılım matris metoduna uygun programlanacaktır. Program çıktıları bilimsel makalelerde çalışılmış teorik ve deneysel sonuçlarla karşılaştırılacaktır.

Anahtar Kelimeler: ince filmler, çok katmanlı, optik film, yazılım, programlama.

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To little beauties Tuğçe and Eda

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A	Absorptance.
B	One of the elements of characteristic matrix of a thin film assembly.
C	One of the elements of characteristic matrix of a thin film assembly.
d	Physical thickness of the layer in a thin film assembly.
E	Electric vector in the electromagnetic field.
H	The magnetic vector in the electromagnetic field.
k	The extinction coefficient.
M	Represents the elements of the characteristic matrix.
N	The complex refractive index. N=n -ik
n	The real part of the refractive index.
R	Reflectance.
T	Transmittance
TE	Transverse electric.
TM	Transverse magnetic.
ϵ	The permittivity of a medium.
η	The tilted optical admittance.
η_s	The tilted admittance of the substrate.
θ	The angle of incidence of in a medium.
λ	The wavelength of light.
ϕ	The phase shift on reflection.

CHAPTER 1

INTRODUCTION

Interference phenomena of light waves occur frequently in nature. Many birds and insects produces colored reflection with their feathers and wings. Oily substance onto water also produce interference patterns and it has been certainly noticed by man since ancient times. The origin of such effects remained unclear untill recent times. The first systemetic study was undertaken by Newton. Newton rings, obtained from multiple reflections of light in a tiny air layer left between a flat and a little convex glass piece. Newton believes that light beams were the propogation of a stream of particles and he rejects the idea of light being a wavelike property. So, this interference effect of light was not properly understood at that moment. In 1960, Huygens proposed that light was a disturbance propogating through the ether as sound moves through the air.

In 1768, Euler advanced the hypothesis that the colors we see depends on the wavelength of the light. In 1801, Young sketched the current theory of color vision in terms of three different (primary) colors. Young's experiments on the interference of two light beams were made around 1800 and published in 1807. They gave the ultimate proof of the wave nature of light and allowed the determination of the wavelength of visible light. Young proposed a few years later that light waves were transverse perturbations of the ether and not longitudinal, as sound waves. The consequences of the finding kept physicists busy for the next hundred years. Young's results were put on a firm mathematical basis by Fresnel. He established the relations between the amplitudes of the reflected and refracted waves and the incident waves, known as the Fresnel formulae [1].

Optical coatings remained a subject of laboratory curiosity in the sense that no industrial applications occurred until the twentieth century, with the notable exception of mirror production. Until the late Middle Ages, mirrors were simply polished metals. At a certain unknown moment, the Venetian glass workers introduced glass silvering using an amalgam of tin and mercury. The method lasted until the nineteenth century, when the backing of glass was made with silver. The development of vacuum apparatus techniques allowed the evaporation of a large class of materials, with the application to optical systems, among others. The methods to deposit thin films in a controllable way increased at a rapid process [1, 2].

Today, advanced electronic and optical devices are manufactured involving single or multilayered structures of materials of very different nature electro-optic and optical materials, semiconductors, insulators, superconductors, and all kinds of oxide and nitride alloys. This rapid development demands accurate deposition methods, characterization, as well as powerful algorithms for fast corrections to predicted performance of the fim systems [1].

Multilayer coatings of thin film are used to modify the optical properties of surfaces. Enhancement or reduction of reflectivity or transmission of mirrors and lenses are well-known examples in the visible region. Coatings are also used as spectral filters and as polarizers and phase retarders. The performance of a multilayer coating is limited by the optical constants of the materials. Coatings can be designed for nearly any specification. Any reflectivity and transmittivity can be obtained by designing multilayered mirrors and lenses to produce any arbitrary reflectivity and transmittivity with respect to wavelength [2].

In principal, determination of the amplitudes and intensities ratio of light refracted, transmitted and absorbed by a thin film or by a multilayer film stack is straightforward and obtained simply by setting up Maxwell's equations and by applying appropriate boundary conditions. But, resulting equations are complicated and evaluations of the properties of given combination of films involve very tedious computation [3, 4].

Characteristic matrix approach is very applicable and easy to manipulate. When designing multilayer stack and calculating the film properties, optical refractive indices, complex optical refractive indices with respect to wavelength and thicknesses of all layer can be placed into characteristic matrix approach easily. For huge number of film layers, computation and simulation of multilayer film stack with characteristic matrix approach provide high speed and has advantages for changing the optical parameters [5].

In order to calculate reflectance, transmittance and absorptance of an optical film stack, Snell's law is used for obtaining the direction of propagation in each of the layers and the Fresnel formulas are used for the amplitude reflection and transmission coefficients at the boundaries between the layers. One assumes that there is no scattering in the volume of a film stack. An incoming wave split into a transmitted and reflected wave at the boundaries [1].

For all material used in this computation, their complex optical refractive indices were obtained from another handbook software. HOC (Handbook of Optical Constants). This software provides spectral optical constants for many type of materials. For most of the optical constants which is used in multilayer computation, they are rearranged and interpolated between 200nm and 1200 nm. Arranged material constants were saved in a regular text form and used for multilayer thin film designs.

This software is developed with Delphi Programming language. It provides excellent opportunities with their visual libraries for designing of user interface. This Delphi programming language is object oriented and uses pascal codes with the additional developed libraries. Complex mathematics library is imported to the program and it is used frequently in functions and procedures. At the end, this program is compiled and exe file is produced. This executable file can work fine with windows operating systems.

In chapter 1, introduction to interference phenomena and thin film concepts is done. In chapter 2, a brief introduction to Maxwell equations, reflection and trasmission concepts and thin film reflectance and transmittance are studied. In chapter 3, extracting matrix elements and expressions for layers, reflectance, transmittance and absorbtance constants of multilayer thin film stack are studied. In chapter 4, developed software inteface is introduced. Capabilities and functionalities of the user interfaces of the program are explained with their pictures. In chapter 5, Functions and procedures used in this developed software are introduced and some programming algorithms are explained with their diagrams and pictures. In chapter 6, outputs of the program are experienced with the studied scientific papers and comparisions are done for different type of the film stacks. In chapter 7, summarization and conlusion are written. At the appendices, Handbook of Optical Constants of Solids (HOC) software is introduced. HOC software interface and their functionalities are expressed with the user interface pictures. Functions of matrix calculations are organized in tables with their Delphi codes. And finally procedures of matrix calculation and procedures for plotting codes are written.

CHAPTER 2

PHYSICAL THEORY

2.1 Maxwell equations

The basics of electricity and magnetism can be summarized as differential forms in four categories:

$$\begin{aligned} \text{Coulomb's Law:} \quad & \nabla \cdot D = \rho && (2.1) \\ \text{Ampere's Law:} \quad & \nabla \times H = J && (2.2) \\ \text{Faraday's Law:} \quad & \nabla \times E + \frac{\partial B}{\partial t} = 0 && (2.3) \\ \text{Absence of free magnetic poles:} \quad & \nabla \cdot B = 0 && (2.4) \end{aligned}$$

Where D is the electric displacement, H the magnetic field vector, E the electric field vector, B the magnetic induction, ρ the electric charge density and J the electric current density.

In addition to these equations, relations between E and D, B and H, E and J can be written as follows:

$$D = \epsilon E \tag{2.5}$$

$$B = \mu H \tag{2.6}$$

$$J = \sigma E \tag{2.7}$$

where ϵ is the dielectric constant, μ the magnetic permeability and σ the conductivity.

Maxwell corrected Ampere's Law by replacing J with $J + \frac{\partial D}{\partial t}$ in equation 2.2 as:

$$\nabla \times H = J + \frac{\partial D}{\partial t} \tag{2.8}$$

In order to obtain plane electromagnetic wave solutions curl of both sides of equation 2.3 must be taken.

$\nabla \times (\nabla \times E) = -\frac{\partial(\nabla \times B)}{\partial t}$ and using identity $\nabla \times (\nabla \times E) = \nabla(\nabla \cdot E) - \nabla^2 E$

After reorganizing and making required changes, it can be rewritten in a proper form as

$$\nabla^2 E = \mu\sigma \frac{\partial E}{\partial t} + \mu\epsilon \frac{\partial^2 E}{\partial t^2} \tag{2.9}$$

If the above steps are applied to the equation 2.2, similar form is obtained as

$$\nabla^2 B = \mu\sigma \frac{\partial B}{\partial t} + \mu\epsilon \frac{\partial^2 B}{\partial t^2} \tag{2.10}$$

Differential solutions of equations 2.9 and 2.10 are of the form

$$E(x,t) = E_0 e^{iw(t - \frac{x}{v})} \tag{2.11}$$

$$B(x,t) = B_0 e^{iw(t - \frac{x}{v})} \tag{2.12}$$

which represents a plane wave of angular frequency ω, travelling along the x-axis with velocity v. We can import phase angle (ϕ) to these equations and can be rewritten as follows:

$$E(x,t) = E_0 e^{i[w(t - \frac{x}{v}) + \phi]} \tag{2.13}$$

$$B(x,t) = B_0 e^{i[w(t - \frac{x}{v}) + \phi]} \tag{2.14}$$

After putting equation 2.13 into equation 2.9, result is obtained as

$$\frac{\omega^2}{v^2} = \omega^2 \epsilon\mu - i\omega\mu\sigma \tag{2.15}$$

In vacum $\sigma = 0$, $v = c$ and $\frac{1}{c^2} = \epsilon_0\mu_0$. Multiply both sides of equation 2.15 with $\frac{c^2}{\omega^2}$. Then equation 2.16 is obtained.

$$\frac{c^2}{v^2} = \frac{\epsilon\mu}{\epsilon_0\mu_0} - i\frac{\mu\sigma}{\epsilon_0\mu_0\omega} \tag{2.16}$$

Here, $\frac{c}{v}$ ratio is dimensionless parameter of the medium, which is denoted by N:

$$N^2 = \frac{\epsilon\mu}{\epsilon_0\mu_0} - i\frac{\mu\sigma}{\epsilon_0\mu_0\omega} \tag{2.17}$$

This implies that N is of the form

$$N = \frac{c}{v} = n - ik \tag{2.18}$$

N is known as the complex refractive index, n is the real part of the refractive index and k is known as the extinction coefficient.

$$N^2 = n^2 - 2ink - k^2 \tag{2.19}$$

and from equation 2.16

$$n^2 - k^2 = \frac{\epsilon\mu}{\epsilon_0\mu_0} \tag{2.20}$$

$$2nk = \frac{\mu\sigma}{\epsilon_0\mu_0\omega} \tag{2.21}$$

By using relations $c = \lambda f$, $f = \frac{\omega}{2\pi}$, $\omega = \frac{2\pi}{\lambda}c$ and $N = \frac{c}{v}$ equation 2.11 can be written as

$$\begin{aligned} E(x,t) &= E_0 e^{i\omega t} e^{-\frac{2i\pi N}{\lambda}x} \\ &= E_0 e^{i\omega t} e^{-\frac{2i\pi(n-ik)}{\lambda}x} \\ &= E_0 e^{i\omega t} e^{-\frac{2i\pi n}{\lambda}x} e^{-\frac{2\pi k}{\lambda}x} \\ &= E_0 e^{-\frac{2\pi k}{\lambda}} e^{i(\omega t - \frac{2\pi n}{\lambda}x)} \end{aligned} \tag{2.22}$$

In equation 2.22 first exponential factor $e^{-\frac{2\pi}{\lambda}kx}$ tells decaying part and the other factor $e^{i(\omega t - \frac{2\pi}{\lambda}nx)}$ tells traveling part. Let the direction of propagation of the wave be given by unit vector $\hat{s}$ where

$$\hat{s} = \alpha i + \beta j + \gamma k \tag{2.23}$$

and where i, j and k are unit vectors along the x, y and z axes, respectively. α, β and γ are cosine factors of the three directions. From equation 2.22

$$\frac{\partial E}{\partial t} = i\omega E \tag{2.24}$$

And from equations 2.5, 2.7 and 2.8

$$\begin{aligned} \nabla \times H &= \sigma E + \epsilon \frac{\partial E}{\partial t} \\ &= (\sigma + i\omega\epsilon)E \\ &= i\frac{\omega N^2}{c^2\mu}E \end{aligned} \tag{2.25}$$

and ∇ product is

$$\nabla = (\frac{\partial}{\partial x}i + \frac{\partial}{\partial y}j + \frac{\partial}{\partial z}k)\times$$

where

$$\frac{\partial}{\partial x} = -i\frac{2\pi N}{c}\alpha = -i\frac{\omega N}{c}\alpha \tag{2.26}$$

$$\frac{\partial}{\partial y} = -i\frac{\omega N}{c}\beta \tag{2.27}$$

$$\frac{\partial}{\partial z} = -i\frac{\omega N}{c}\gamma \tag{2.28}$$

so that

$$\nabla \times H = -i\frac{\omega N}{c}(\hat{s} \times H) \tag{2.29}$$

Then

$$-i\frac{\omega N}{c}(\hat{s}\times H) = i\frac{\omega N^2}{c^2\mu}E \tag{2.30}$$

So

$$(\hat{s}\times H) = -\frac{N}{c\mu}E \tag{2.31}$$

and similarly

$$\frac{N}{c\mu}(\hat{s}\times E) = H \tag{2.32}$$

Hence, E, H and $\hat{s}$ are mutually perpendicular and form right-handed set. The quantity $N/c\mu$ has the dimensions of an admittance and is known as the characteristic optical admittance of the medium, denoted as y. And admittance of free space ($\mathcal{Y}$) is given by

$$\mathcal{Y} = (\epsilon_0/\mu_0)^{1/2} = 2.6544x10^{-3} \tag{2.33}$$

Admittance of any medium can be written as

$$y = N\mathcal{Y} \tag{2.34}$$

and

$$H = y(\hat{s}\times E) = N\mathcal{Y}(\hat{s}\times E) \tag{2.35}$$

2.2 Simple Boundary

Thin film filters usually consist of a number of boundaries between various homegenous media and calculations are affected by these boundaries. A single boundary is the simplest one as seen in Figure 2.1. Consider absorbtion free media, i.e. $k = 0$. At a boundary, tangential components of E and H are continuous across it. In this case boundary is defined by $z = 0$, and the tangential components must be continuous for all values of x, y, and t.

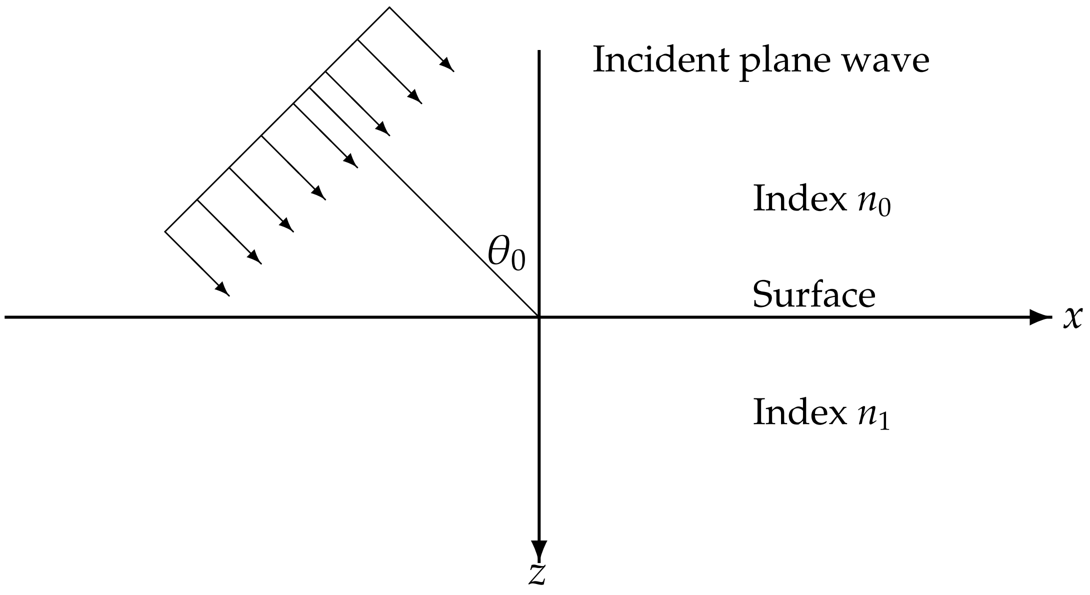


Figure 2.1: Plane wave incident on a single surface.

Let the direction cosines of the $\hat{s}$ vectors of the transmitted and reflected waves be $(\alpha_t, \beta_t, \gamma_t)$ and $(\alpha_r, \beta_r, \gamma_r)$ respectively. So phase factors can be written in the form :

$$\text{Incident wave:} \qquad e^{i[\omega_i t - (\frac{2\pi n_0}{\lambda_i})(x \sin\vartheta_0 + z\cos\vartheta_0)]} \tag{2.36}$$

$$\text{Reflected wave:} \qquad e^{i[\omega_r t - (\frac{2\pi n_0}{\lambda_r})(\alpha_r x + \beta_r y + \gamma_r z)]} \tag{2.37}$$

$$\text{Transmitted wave:} \qquad e^{i[\omega_i t - (\frac{2\pi n_0}{\lambda_i})(\alpha_t x + \beta_t y + \gamma_t z)]} \tag{2.38}$$

The relative phases of these waves are included in the complex amplitudes. Satisfying boundary conditions for all x, y, t at $z = 0$ implies that the coefficients of these variables must be identically equal:

$$\omega \equiv \omega_r \equiv \omega_t \tag{2.39}$$

that is, there is no change of frequency and also free space wavelength is equal:

$$\lambda \equiv \lambda_r \equiv \lambda_t \tag{2.40}$$

Next

$$0 \equiv n_0\beta_r \equiv n_1\beta_t \tag{2.41}$$

that is, the directions of the reflected and transmitted beams are confined to plane of incidence. This means that the direction cosines of the reflected and transmitted waves are of the form:

$$\alpha = \sin\vartheta \qquad \text{and} \qquad \gamma = \cos\vartheta \tag{2.42}$$

Also

$$n_0 \sin\vartheta_0 \equiv n_0\alpha_r \equiv n_1\alpha_t \tag{2.43}$$

$$n_0 \sin \vartheta_0 = n_0 \sin \vartheta_r = n_1 \sin \vartheta_t \tag{2.44}$$

Here $\vartheta_0 = \vartheta_r$ is the law of refraction and

$$n_0 \sin \vartheta_0 = n_1 \sin \vartheta_t \qquad \text{Snell's Law} \tag{2.45}$$

2.3 Normal Incidence

Let us limit initial discussion to normal incidence and let the incident wave be a plane-polarized plane harmonic wave. The coordinate axes are shown in Figure 2.2. The xy plane is plane of boundary and incident wave is propagating along the z axis. E vector is along the x axis and H vector is along the y axis.

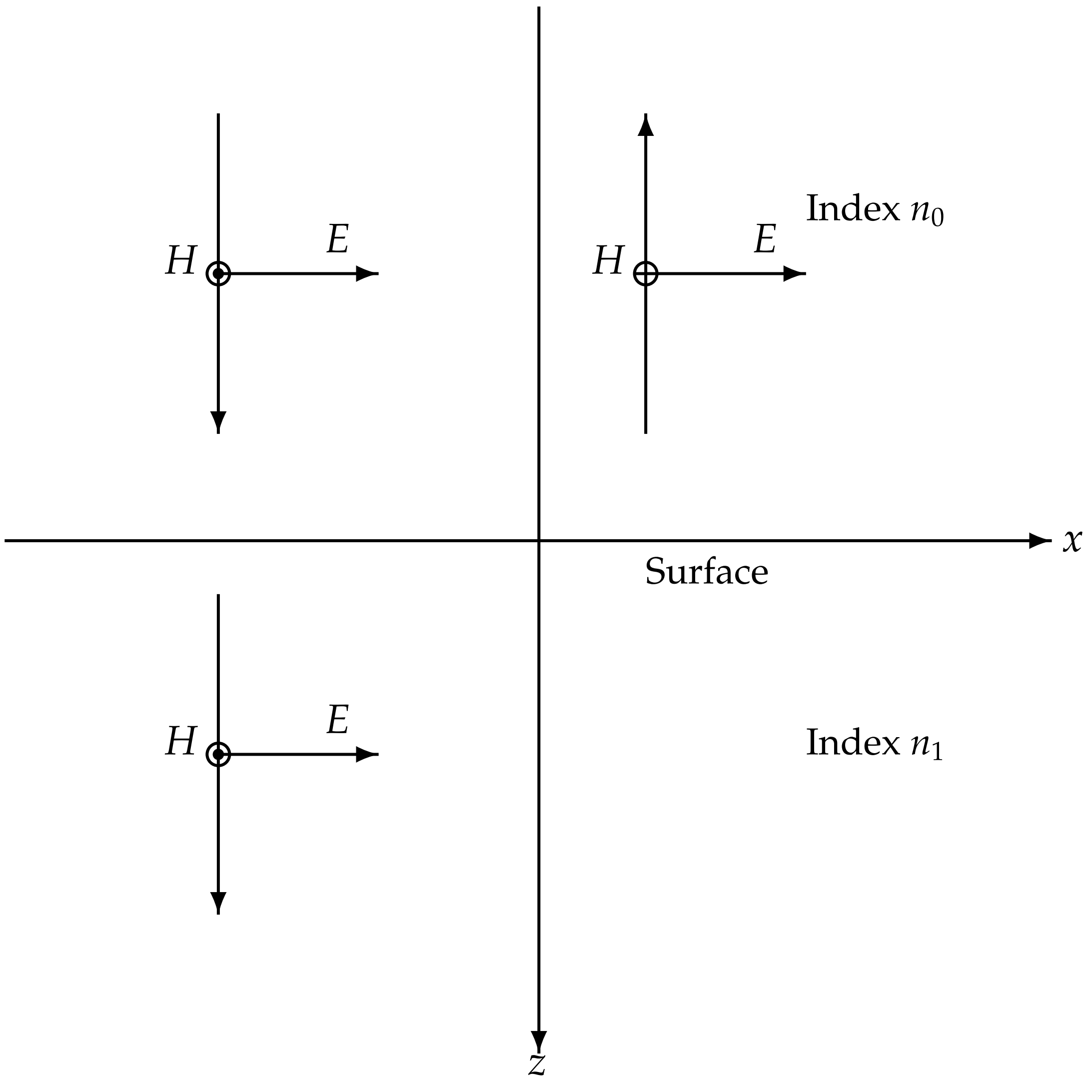


Figure 2.2: Convention defining positive directions of the electric and magnetic vectors for reflection and transmission at an interface at normal incidence.

(a) Electric vectors continuous across the boundary:

$$E_i + E_r = E_t \tag{2.46}$$

(b) Magnetic vector continuous across the boundary:

$$H_i - H_r = H_t \tag{2.47}$$

The relationship between magnetic and electric field through the characteristic admittance gives:

$$y_0 E_i - y_0 E_r = y_1 E_t \tag{2.48}$$

E_t can be eliminated to give

$$y_1(E_i + E_r) = y_0(E_i - E_r) \tag{2.49}$$

i.e.

$$\frac{E_r}{E_i} = \frac{y_0 - y_1}{y_0 + y_1} = \frac{n_0 - n_1}{n_0 + n_1} \tag{2.50}$$

similarly, eliminating E_r,

$$\frac{E_t}{E_i} = \frac{2y_0}{y_0 + y_1} = \frac{2n_0}{n_0 + n_1} \tag{2.51}$$

These quantities are called as the amplitude of reflection and transmission coefficients and are denoted by ρ and τ respectively. Thus

$$\rho = \frac{y_0 - y_1}{y_0 + y_1} = \frac{n_0 - n_1}{n_0 + n_1} \tag{2.52}$$

$$\tau = \frac{2y_0}{y_0 + y_1} = \frac{2n_0}{n_0 + n_1} \tag{2.53}$$

2.4 Oblique Incidence

There are two orientations of the incident wave. The vector electrical amplitudes aligned in the plane of incidence and the vector electrical amplitudes aligned normal to the plane of incidence. In each of these cases, the orientations of the transmitted and reflected vector amplitudes are the same as for the incident wave. A wave with the electric vector in the plane of incidence is known as p-polarized or, sometimes, TM(transfer magnetic) and a wave with the electric vector normal to the plane of incidence as s-polarized or,sometimes, TE(transfer electric).

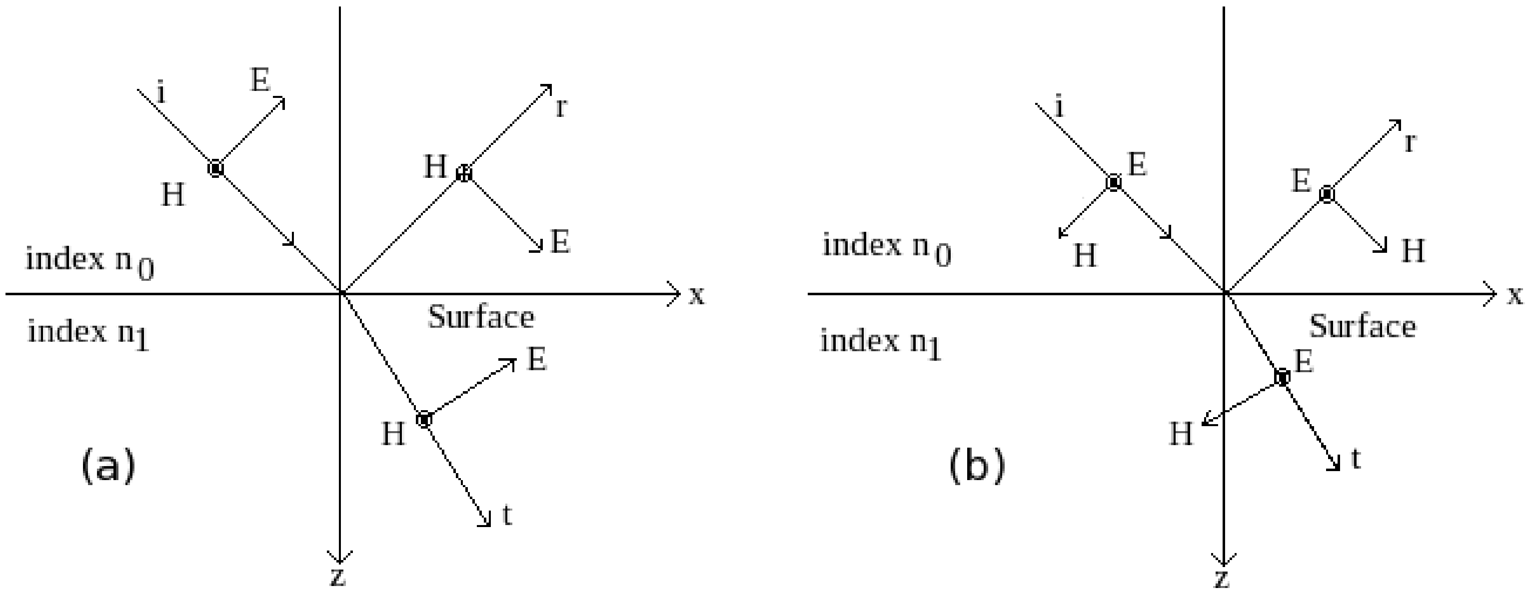


Figure 2.3: (a) Convention defining of positive directions of the electric and magnetic vectors for p-polarized light (b) Convention defining of positive directions of the electric and magnetic vectors for s-polarized light.

2.4.1 p-polarized light

(a) Electric component parallel to the boundary, continuous across it:

$$E_i \cos \vartheta_0 + E_r \cos \vartheta_0 = E_t \cos \vartheta_1 \tag{2.54}$$

(b) Magnetic component parallel to the boundary and continuous across it. Since $H = yE$

$$y_0 E_i - y_0 E_r = y_1 E_t \tag{2.55}$$

By introducing new variables for E and H and in a convenient orientation form:

$$\mathbb{E}_i = E_i \cos \vartheta_0 \qquad \mathbb{H}_i = \frac{y_0}{\cos \vartheta_0} \mathbb{E}_i \tag{2.56}$$

$$\mathbb{E}_r = E_r \cos \vartheta_0 \qquad \mathbb{H}_r = \frac{y_0}{\cos \vartheta_0} \mathbb{E}_r \tag{2.57}$$

$$\mathbb{E}_t = E_t \cos \vartheta_1 \qquad \mathbb{H}_t = \frac{y_1}{\cos \vartheta_1} \mathbb{E}_t \tag{2.58}$$

Hence (a) Electric field parallel to the boundary:

$$\mathbb{E}_i + \mathbb{E}_r = \mathbb{E}_t \tag{2.59}$$

(b) Magnetic field parallel to the boundary:

$$\frac{y_0}{\cos \vartheta_0} \mathbb{H}_i - \frac{y_0}{\cos \vartheta_0} \mathbb{H}_r = \frac{y_1}{\cos \vartheta_1} \mathbb{H}_t \tag{2.60}$$

And then

$$\rho_p = \frac{\mathbb{E}_r}{\mathbb{E}_i} = \frac{(y_0 / \cos \vartheta_0 - y_1 / \cos \vartheta_1}{y_0 / \cos \vartheta_0 + y_1 / \cos \vartheta_1} \tag{2.61}$$

$$\tau_p = \frac{\mathbb{E}_t}{\mathbb{E}_i} = \frac{2\frac{y_0}{\cos\vartheta_0}}{(\frac{y_0}{\cos\vartheta_0} + \frac{y_1}{\cos\vartheta_1})} \tag{2.62}$$

Hence reflectance and transmittance

$$R_p = \frac{(\frac{y_0}{\cos\vartheta_0} - \frac{y_1}{\cos\vartheta_1})^2}{(\frac{y_0}{\cos\vartheta_0} + \frac{y_1}{\cos\vartheta_1})^2} \tag{2.63}$$

$$T_p = \frac{\frac{4y_0 y_1}{\cos\vartheta_0\cos\vartheta_1}}{(\frac{y_0}{\cos\vartheta_0} + \frac{y_1}{\cos\vartheta_1})^2} \tag{2.64}$$

2.4.2 s-polarized light

In case of s-polarization the amplitudes of the components of the waves parallel to the boundary are

$$\mathbb{E}_i = E_i \qquad \mathbb{H}_i = H_i\cos\vartheta_0 = y_0\cos\vartheta_0\mathbb{E}_i \tag{2.65}$$

$$\mathbb{E}_r = E_r \qquad \mathbb{H}_r = H_r\cos\vartheta_0 = y_0\cos\vartheta_0\mathbb{E}_r \tag{2.66}$$

$$\mathbb{E}_t = E_t \qquad \mathbb{H}_t = H_t\cos\vartheta_1 = y_1\cos\vartheta_1\mathbb{E}_t \tag{2.67}$$

And similar analysis leads to

$$\rho_s = \frac{\mathbb{E}_r}{\mathbb{E}_i} = \frac{y_0\cos\vartheta_0 - y_1\cos\vartheta_1}{y_0\cos\vartheta_0 + y_0\cos\vartheta_0} \tag{2.68}$$

$$\tau_s = \frac{\mathbb{E}_t}{\mathbb{E}_i} = \frac{2y_0\cos\vartheta_0}{y_0\cos\vartheta_0 + y_1\cos\vartheta_1} \tag{2.69}$$

Hence reflectance and transmittance are

$$R_s = \frac{(y_0\cos\vartheta_0 - y_1\cos\vartheta_1)^2}{(y_0\cos\vartheta_0 + y_1\cos\vartheta_1)^2} \tag{2.70}$$

$$T_s = \frac{4y_0\cos\vartheta_0 y_1\cos\vartheta_1}{(y_0\cos\vartheta_0 + y_1\cos\vartheta_1)^2} \tag{2.71}$$

2.5 Oblique Incidence in Absorbing Media

Phase factors can be written as

$$\text{Incident}: \quad e^{i[\omega t - \frac{2\pi n_0}{\lambda}(x\sin\vartheta_0 + z\cos\vartheta_0)]} \tag{2.72}$$

$$\text{Reflected}: \quad e^{i[\omega t - \frac{2\pi n_0}{\lambda}(x\sin\vartheta_0 - z\cos\vartheta_0)]} \tag{2.73}$$

$$\text{Transmitted}: \quad e^{i[\omega t - \frac{2\pi(n_1 - ik_1)}{\lambda}(\alpha x + \gamma z)]} \tag{2.74}$$

where α and γ in the transmitted phase factors are the only unknowns. The phase factor must be identically equal for all x and t with $z = 0$. This implies

$$\alpha = \frac{n_0 \sin \vartheta_0}{n_1 - ik_1} \tag{2.75}$$

and, since $\alpha^2 + \gamma^2 = 1$

$$\gamma = (1 - \alpha^2)^{1/2} \tag{2.76}$$

And solutions to this equation,

$$\begin{aligned} (n_1 - ik_1)\gamma &= [(n_1 - ik_1)^2 - n_0^2 \sin^2 \vartheta_0]^{1/2} \\ &= [n_1^2 - k_1^2 - n_0^2 \sin^2 \vartheta_0 - i2n_1k_1]^{1/2} \end{aligned} \tag{2.77}$$

And transmitted phase factor is of the form

$$e^{i[\omega t - (2\pi n_0 \sin \vartheta_0 x/\lambda) - (2\pi/\lambda)(a - ib)z]} = e^{(-2\pi bz/\lambda)} e^{i[\omega t - (2\pi n_0 \sin \vartheta_0 x/\lambda) - (2\pi az/\lambda)]} \tag{2.78}$$

where

$$(a - ib) = [n_1^2 - k_1^2 - n_0^2 \sin^2 \vartheta_0 - 2in_1k_1]^{1/2} \tag{2.79}$$

A wave having such a this type of phase factor is known as inhomegeneous. While propagating along the z axis, amplitude of the wave decreases. Including complex angles

$$\begin{aligned} (n_1 - ik_1) \sin \vartheta_1 &= n_0 \sin \vartheta_0 && (2.80) \\ \alpha &= \sin \vartheta_1 && (2.81) \\ \gamma &= \cos \vartheta_1 && (2.82) \\ (a - ib) &= (n_1 - ik_1) \cos \vartheta_1 && (2.83) \end{aligned}$$

The calculation of amplitudes

$$\begin{aligned} \nabla &\equiv (\frac{\partial}{\partial x} i + \frac{\partial}{\partial y} j + \frac{\partial}{\partial z} k) \times \\ &\equiv (-i\frac{2\pi N}{\lambda}\alpha i - i\frac{2\pi N}{\lambda}\gamma k) \times \end{aligned}$$

For p-waves the H vector is parallel to the boundary in the y direction and so $H = H_y j$. The component of E parallel to the boundary will then be in the x direction, $E_x i$.

$$\begin{aligned} \nabla \times H &= \sigma E + \epsilon \frac{\partial E}{\partial t} \\ &= (\sigma + i\omega\epsilon)E \\ &= \frac{i\omega N^2}{c^2 \mu} E \end{aligned} \tag{2.84}$$

Tangential component of the $\nabla \times H$ is in the x direction so that

$$-i\frac{2\pi N}{\lambda}\gamma(k \times j)H_y = i\frac{\omega N^2}{c^2\mu}E_x i \tag{2.85}$$

But $-(k \times j) = i$ and so that

$$\begin{aligned} \eta_p &= \frac{H_y}{E_x} = \frac{\omega N \lambda}{2\pi c^2 \mu\gamma} = \frac{N}{c\mu\gamma} \\ &= \frac{N\Upsilon}{\gamma} = \frac{y}{\gamma} \end{aligned} \tag{2.86}$$

For s-waves

$$\nabla \times E = \frac{\partial B}{\partial t} = -\mu\frac{\partial H}{\partial t} \tag{2.87}$$

E is along the y axis and a similar analysis gives:

$$\eta_s = \frac{H_x}{E_y} = N\Upsilon\gamma = y\gamma \tag{2.88}$$

Now γ can be identified as $\cos\vartheta$, provided that ϑ is permitted to be complex, and so

$$\eta_p = y/\cos\vartheta \tag{2.89}$$

$$\eta_s = y\cos\vartheta \tag{2.90}$$

Thus the amplitude reflection and transmission coefficients

$$\rho = \frac{\eta_0 - \eta_1}{\eta_0 - \eta_1} \tag{2.91}$$

$$\tau = \frac{2\eta_0}{\eta_0 + \eta_1} \tag{2.92}$$

and reflectance and transmittance become as [4, 6, 7]:

$$R = \left(\frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\right)\left(\frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\right)^* \tag{2.93}$$

$$T = \frac{4\eta_0 Re(\eta_1)}{(\eta_0 - \eta_1)(\eta_0 - \eta_1)^*} \tag{2.94}$$

CHAPTER 3

MATRIX METHOD FOR MULTILAYER THIN FILM

Multilayer thin film stack is obtained by deposition of more than one type of materials to top of other layer starting from the substrate. Each of the layers has a physical thickness t_m and optical constants given by $N_m = n_m - ik_m$, where n_m is the dispersive refractive index related to the velocity and k_m is the dispersive extinction coefficient related to the decaying of the oscillation amplitude of the incident electric field.

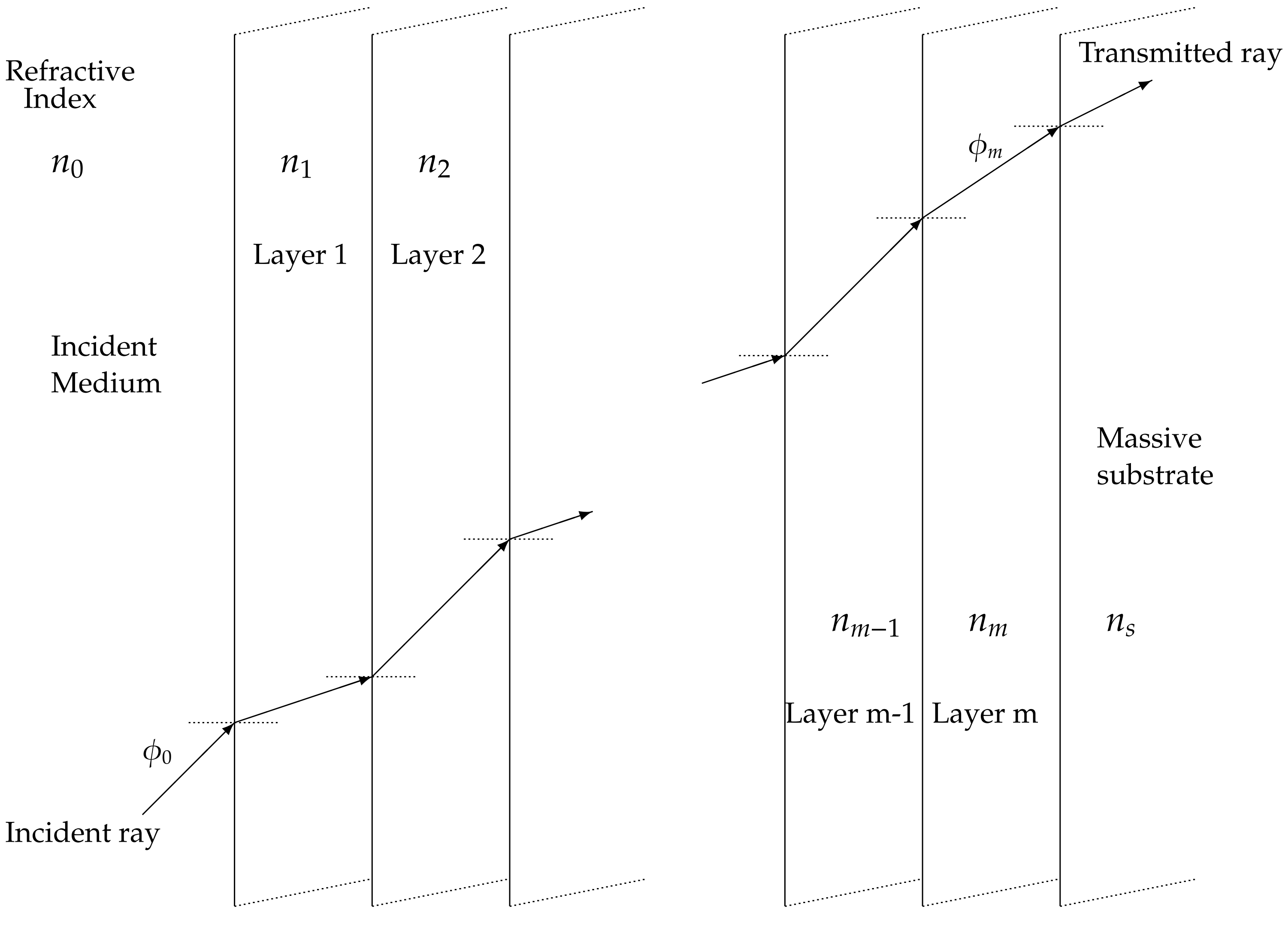


Figure 3.1: Film stack.

An ideal multilayer stack is shown in Figure 3.1. Each layer in the stack has three parameters t_m, n_m and k_m. Besides these, there are additional parameters n_s, k_s coming from the substrate and n_0, refractive index of air or medium that contacts with the top layer of the multilayer stack. When electromagnetic radiation travels from one boundary to the next boundary, a phase difference occurs and it is expressed for m^{th} layer as $\delta_m = \frac{2\pi}{\lambda} N_m t_m$.

When electromagnetic radiation is incident upon a multilayer stack at oblique incidence, both R and T must be computed seperately with respect to the plane of polarization and average reflectance and average transmittance can be obtained by taking the mean of the two polarizations (i.e. $R_{avg} = \frac{1}{2}(R_s + R_p)$ and $T_{avg} = \frac{1}{2}(T_s + T_p)$).

3.1 Extracting Matrix Elements

The calculation matrix described here, determines the spectral transmittance and reflectance profiles for a loss-free multilayer design on an absorptive substrate.

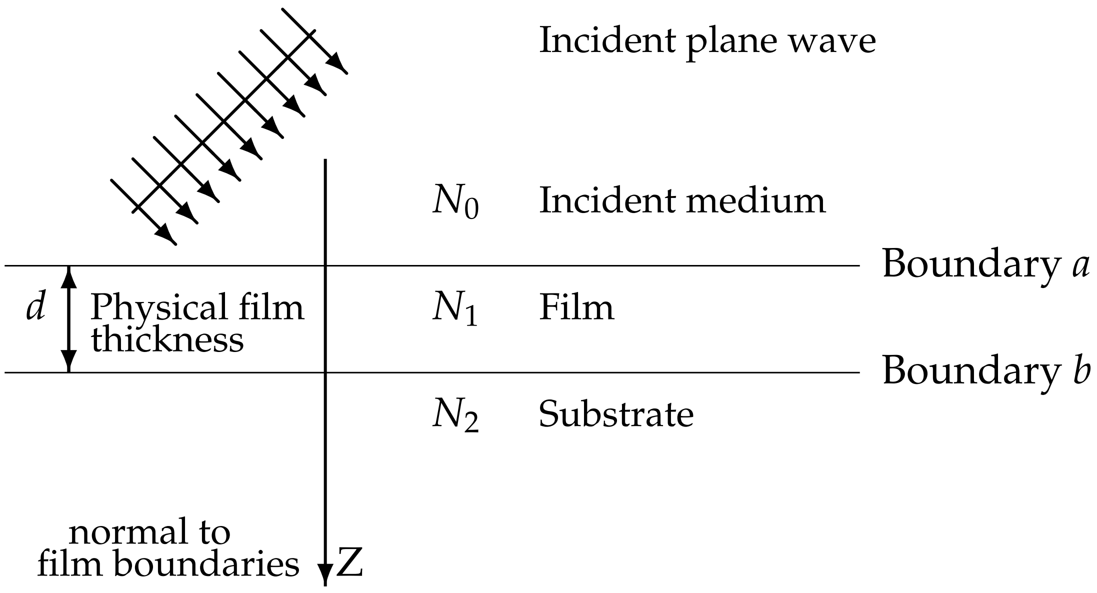


Figure 3.2: Plane wave incident on a single film.

The electric and magnetic field vectors travelling in the direction of incidence are denoted by (+) sign, and travelling opposite in direction of incidence are denoted by (-) minus sign.

The matrix is calculated at each boundary throughout the multilayer and terms of matrix changes with the properties of the layers. Tangential component of the electric (E) and magnetic field (H) vectors must be continuous at each boundary. By considering Figure 3.2, at the interface of the layer, the tangential components of E and H are:

$$\begin{aligned} E_b &= E_{1b}^+ + E_{1b}^- && (3.1) \\ H_b &= \eta_1 E_{1b}^+ - \eta_1 E_{1b}^- && (3.2) \end{aligned}$$

Common phase factors are neglected and E_b and H_b are rewritten as:

$$\begin{aligned} E_{1b}^+ &= \frac{1}{2}(H_b/\eta_1 + E_b) && (3.3) \\ E_{1b}^- &= \frac{1}{2}(-H_b/\eta_1 + E_b) && (3.4) \\ H_{1b}^+ &= \eta_1 E_{1b}^+ = \frac{1}{2}(H_b + \eta_1 E_b) && (3.5) \\ H_{1b}^+ &= -\eta_1 E_{1b}^- = \frac{1}{2}(H_b - \eta_1 E_b) && (3.6) \end{aligned}$$

The phase factor of the positive-going wave is multiplied by $\exp(i\delta)$ where $\delta = 2\pi N_1 d \cos \nu_1/\lambda$, for negative-going wave, it is multiplied by $\exp(-i\delta)$. This procedure is valid when the film is thin. The values of E and H at the interface are expressed as:

$$\begin{aligned} E_{1a}^+ &= E_{1b}^+ e^{i\delta} = \frac{1}{2}(H_b/\eta_1 + E_b)e^{i\delta} && (3.7) \\ E_{1a}^- &= E_{1b}^+ e^{-i\delta} = \frac{1}{2}(-H_b/\eta_1 + E_b)e^{i\delta} && (3.8) \\ H_{1a}^+ &= H_{1b}^+ e^{i\delta} = \frac{1}{2}(H_b + \eta_1 E_b)e^{i\delta} && (3.9) \\ H_{1a}^- &= H_{1b}^- e^{-i\delta} = \frac{1}{2}(H_b - \eta_1 E_b)e^{-i\delta} && (3.10) \end{aligned}$$

So that

$$\begin{aligned} E_a &= E_{1a}^+ + E_{1a}^- && (3.11) \\ &= E_b\left(\frac{e^{i\delta} + e^{-i\delta}}{2}\right) + H_b\left(\frac{e^{i\delta} - e^{-i\delta}}{2\eta_1}\right) && (3.12) \\ &= E_b \cos\delta + H_b \frac{i \sin\delta}{\eta_1} && (3.13) \\ H_a &= H_{1a}^+ + H_{1a}^- && (3.14) \\ &= E_b \eta_1 \left(\frac{e^{i\delta} - e^{-i\delta}}{2}\right) + H_b\left(\frac{e^{i\delta} + e^{-i\delta}}{2}\right) && (3.15) \\ &= E_b i\eta_1 \sin\delta + H_b \cos\delta && (3.16) \end{aligned}$$

This can be written in the form of matrix notation as:

$$\begin{bmatrix} E_a \\ H_a \end{bmatrix} = \begin{bmatrix} \cos(\delta_1) & (i \sin(\delta_1)/\eta_1) \\ i\eta_1 \sin(\delta_1) & \cos(\delta_1) \end{bmatrix} \begin{bmatrix} E_b \\ H_b \end{bmatrix} \qquad (3.17)$$

Where: $\delta_1 = 2\pi N_1 d_1 \cos(\theta_1)/\lambda$, d is the physical thickness, θ is the incident angle and N is the complex refractive index of the layer, η is the optical admittance given by $\eta = y(n - ik)$ for the layer material and y is the admittance of free space given as $y = \sqrt{\varepsilon_0/\mu_0} = 0.002654$, [2, 5, 8].

3.2 Multilayer Calculation Including Layer Absorption

For absorbing layers refractive indices are replaced by complex dispersive quantities and complex Fresnel coefficients are obtained. The relation between electric and magnetic vectors for a single film in the matrix form is as follows:

$$\begin{bmatrix} E_a \\ H_b \end{bmatrix} = \begin{bmatrix} \cos(\delta_1) & (i\sin(\delta_1))/\eta_1 \\ i\eta_1 \sin(\delta_1) & \cos(\delta_1) \end{bmatrix} \begin{bmatrix} E_b \\ H_b \end{bmatrix} \tag{3.18}$$

where, a is the incident medium boundary and b is the substrate boundary. $\eta = H/E$ and matrix can be rewritten as

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} \cos(\delta_1) & (i\sin(\delta_1))/\eta_1 \\ i\eta_1 \sin(\delta_1) & \cos(\delta_1) \end{bmatrix} \begin{bmatrix} 1 \\ \eta_2 \end{bmatrix} \tag{3.19}$$

Here B = normalized electric field amplitude and C = normalized magnetic field amplitude.

This recursive matrix can be extended to the general case of an assembly of q-layers.

$$\begin{bmatrix} B \\ C \end{bmatrix} = \prod_{m=1}^{q} \begin{bmatrix} \cos(\delta_m) & (i\sin(\delta_m))/\eta_m \\ i\eta_m \sin(\delta_m) & \cos(\delta_m) \end{bmatrix} \begin{bmatrix} 1 \\ \eta_s \end{bmatrix} \tag{3.20}$$

where the phase factor $\delta_m = 2\pi N_m d_m \cos(\theta_m)/\lambda$ and $\eta_s = y(n_s - ik_s)$ for the substrate.

$$\eta_m = yN_m \cos(\theta_m) \quad \text{for s-polarization (TE)} \tag{3.21}$$

$$\eta_m = \frac{yN_m}{\cos(\theta_m)} \quad \text{for p-polarization (TM)} \tag{3.22}$$

For exit medium or substrate:

$$\eta_s = yN_s \cos(\theta_s) \quad \text{for s-polarization (TE)} \tag{3.23}$$

$$\eta_s = \frac{yN_s}{\cos(\theta_s)} \quad \text{for p-polarization (TM)} \tag{3.24}$$

Angles θ_m and θ_s can be found with the help of Snell's Law.

$$N_0 \sin(\theta_0) = N_m \sin(\theta_m) = N_s \sin(\theta_s) \tag{3.25}$$

By using the admittance of the incident medium η_0, the reflectance, transmittance and absorbtance can be written as:

$$R_q = \left(\frac{\eta_0 B - C}{\eta_0 B + C}\right)\left(\frac{\eta_0 B - C}{\eta_0 B + C}\right)^* \tag{3.26}$$

$$T_q = \frac{4\eta_0 Re(\eta_s)}{(\eta_0 B + C)(\eta_0 B + C)^*} \tag{3.27}$$

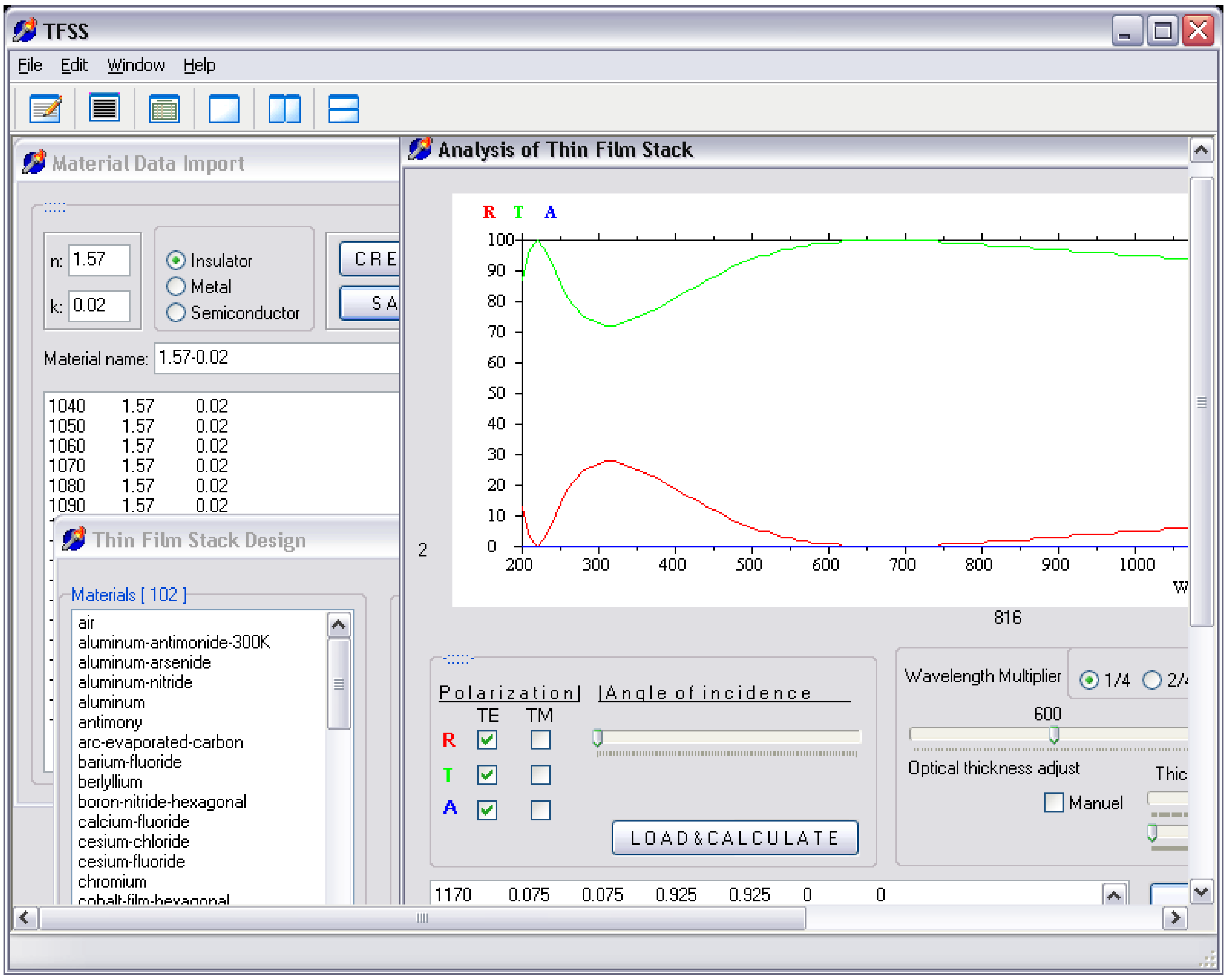
$$A_q = \frac{4\eta_0 Re(BC^* - \eta_s)}{(\eta_0 B + C)(\eta_0 B + C)^*} \tag{3.28}$$

Here, reflectance is the ratio of energy coming from the surface of the outer layer to the medium, transmittance is the ratio of energy that coming to the substrate surface and absorptance is the ratio of energy loss while passing through the film stack [2, 4, 5, 8, 9].

CHAPTER 4

USER INTERFACE OF THE SOFTWARE

The developed software has useful graphical user interface. It is divided into three parts. First part is about data importing interface, second part is about film stack design and the last part is about analysing of the thin film stack.



n: 1.57
k: 0.02
● Insulator
○ Metal
○ Semiconductor
Material name: 1.57-0.02

```
1040   1.57   0.02
1050   1.57   0.02
1060   1.57   0.02
1070   1.57   0.02
1080   1.57   0.02
1090   1.57   0.02
```

Materials [102]
air
aluminum-antimonide-300K
aluminum-arsenide
aluminum-nitride
aluminum
antimony
arc-evaporated-carbon
barium-fluoride
berlyllium
boron-nitride-hexagonal
calcium-fluoride
cesium-chloride
cesium-fluoride
chromium
cobalt-film-hexagonal

Polarization
Angle of incidence

	TE	TM
R	☑	☐
T	☑	☐
A	☑	☐

Wavelength Multiplier ● 1/4 ○ 2/
Optical thickness adjust
☐ Manuel

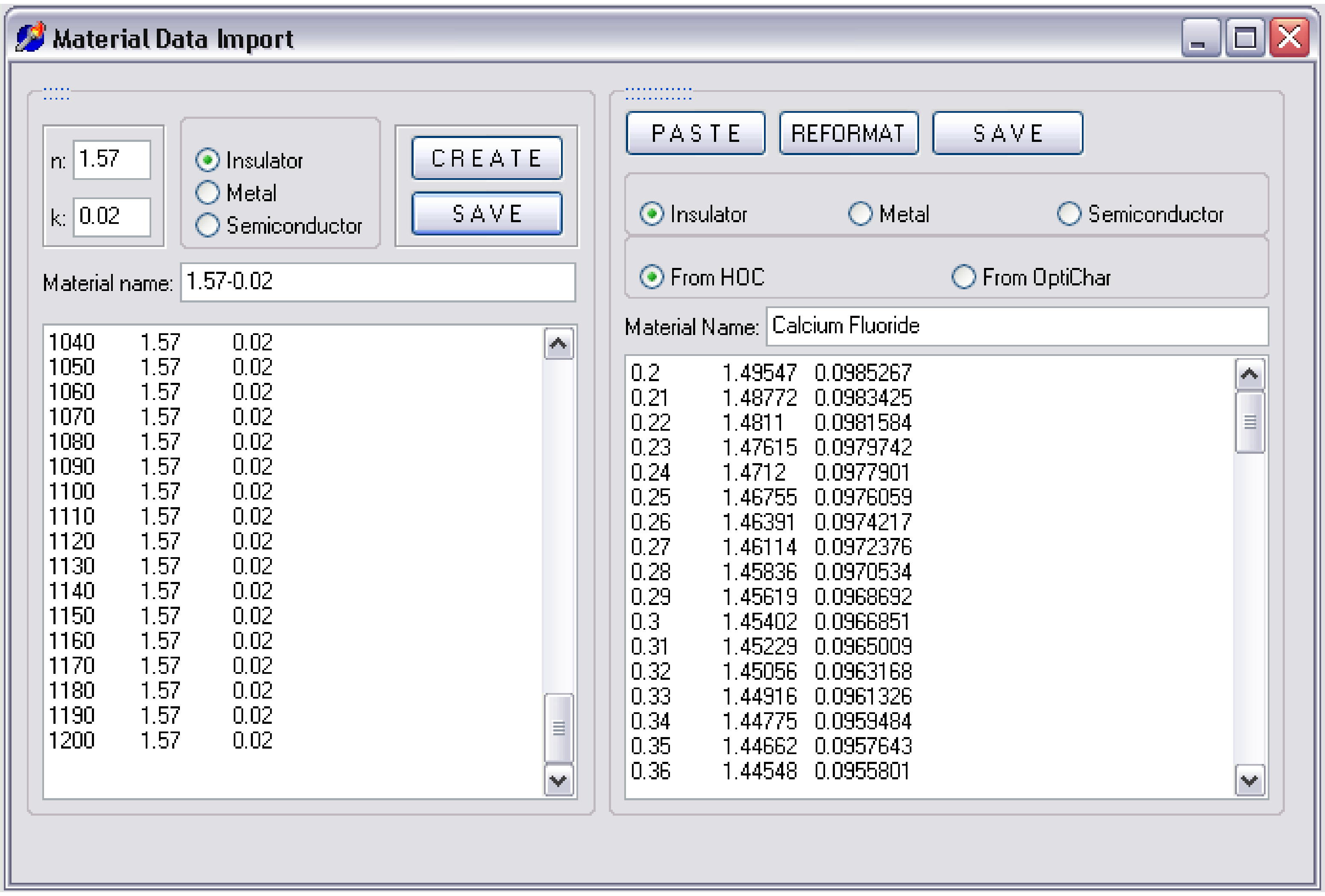
```
1170   0.075   0.075   0.925   0.925   0   0
```

Figure 4.1: Print screen of all three sub program interfaces.

All three parts have their own functionals. Design interface and analyis interface work as coordinated. On the contrary data importing part works stand alone. All three interfaces are displayed in the frame of main program as seen in Figure 4.1.

4.1 Data Importing Interface

Data importing interface is used for data creating, importing and manipulation. This section is divided into two main parts as seen in Figure 4.2. The left part is used for creating arbitrary data by entering the desired constants to editbox, refractive index n and extinction coefficient k with respect to wavelength. User can also classify the arbitrary data as insulator, metal or semiconductor. This classification gives usefulness to program. Once the data is created, it can be saved as text document file under the materials folder by clicking the save button.



n: 1.57
k: 0.02

● Insulator
○ Metal
○ Semiconductor

Material name: 1.57-0.02

```
1040    1.57    0.02
1050    1.57    0.02
1060    1.57    0.02
1070    1.57    0.02
1080    1.57    0.02
1090    1.57    0.02
1100    1.57    0.02
1110    1.57    0.02
1120    1.57    0.02
1130    1.57    0.02
1140    1.57    0.02
1150    1.57    0.02
1160    1.57    0.02
1170    1.57    0.02
1180    1.57    0.02
1190    1.57    0.02
1200    1.57    0.02
```

● Insulator ○ Metal ○ Semiconductor

● From HOC ○ From OptiChar

Material Name: Calcium Fluoride

```
0.2     1.49547  0.0985267
0.21    1.48772  0.0983425
0.22    1.4811   0.0981584
0.23    1.47615  0.0979742
0.24    1.4712   0.0977901
0.25    1.46755  0.0976059
0.26    1.46391  0.0974217
0.27    1.46114  0.0972376
0.28    1.45836  0.0970534
0.29    1.45619  0.0968692
0.3     1.45402  0.0966851
0.31    1.45229  0.0965009
0.32    1.45056  0.0963168
0.33    1.44916  0.0961326
0.34    1.44775  0.0959484
0.35    1.44662  0.0957643
0.36    1.44548  0.0955801
```

Figure 4.2: Print screen of the data import interface.

The right side of the program is used generally for data obtained from other softwares, Handbook of Optical Constants *HOC* and OptiChar. From HOC, interpolated data can be obtained by using functionality of HOC and after copying as regular text from its interface, one can insert data to right part interface by clicking to paste button. This pasted data has not a proper format. So it must be reformatted. This is done by clicking the reformat button and wavelength is converted into nanometer and extra spaces are trimmed and parameters are separeted by inserting 'tab' character between them. Nonetheless, data which is obtained from optichar has only trimming for extra spaces and needs seperating parameters by 'tab' character. This 'tab' character is used for explotation which will be used for other procedures to seperate parameters again.

4.2 Thin Film Stack Design Interface

Thin film stack design is begin with adding layers over the substrate. See Figure 4.3. The last added layer is the outer one. Materials saved as text files before are stored in a listbox placed at the left of the interface. This material listbox has two main functionlities, 'adding layers to stack' and 'setting the selected material as a substrate'. A single selection or multiple selection is possible and they are added as layers to stack by right click procedures. Any material can be selected as a substrate again with right click procedures.

The next listbox titled as Film Design is used for storing layers and it has also right click procedures in order to make manipulation over layer lists.

The chart on the right side is used for graphing the materials parameters. When material is selected in the material listbox, it is graphed with the help of delphi component.

After finishing the film design, in order to complate the last proceudre, 'SET' button must be clicked. At this step, all materials parameters are loaded into an array, in other words, they are transferred to RAM from hard drive. The aim of this transformation is getting more speed while arranging the parameters to arrays. Because reading from RAM is more faster than the hard drive. According to ordering designed situations, material paremeters are exploted and placed into the three dimensional array which will be used for simulation.

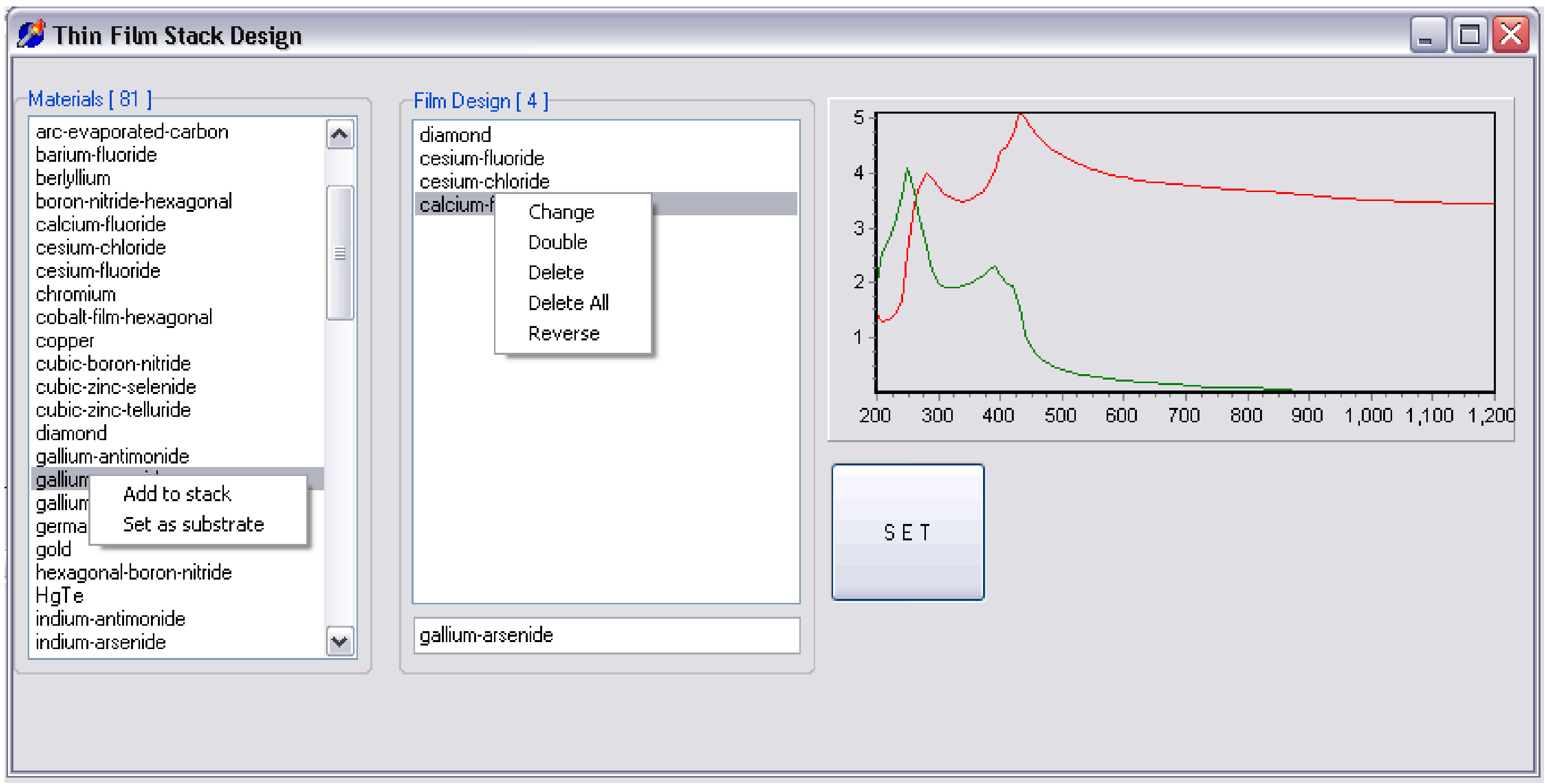
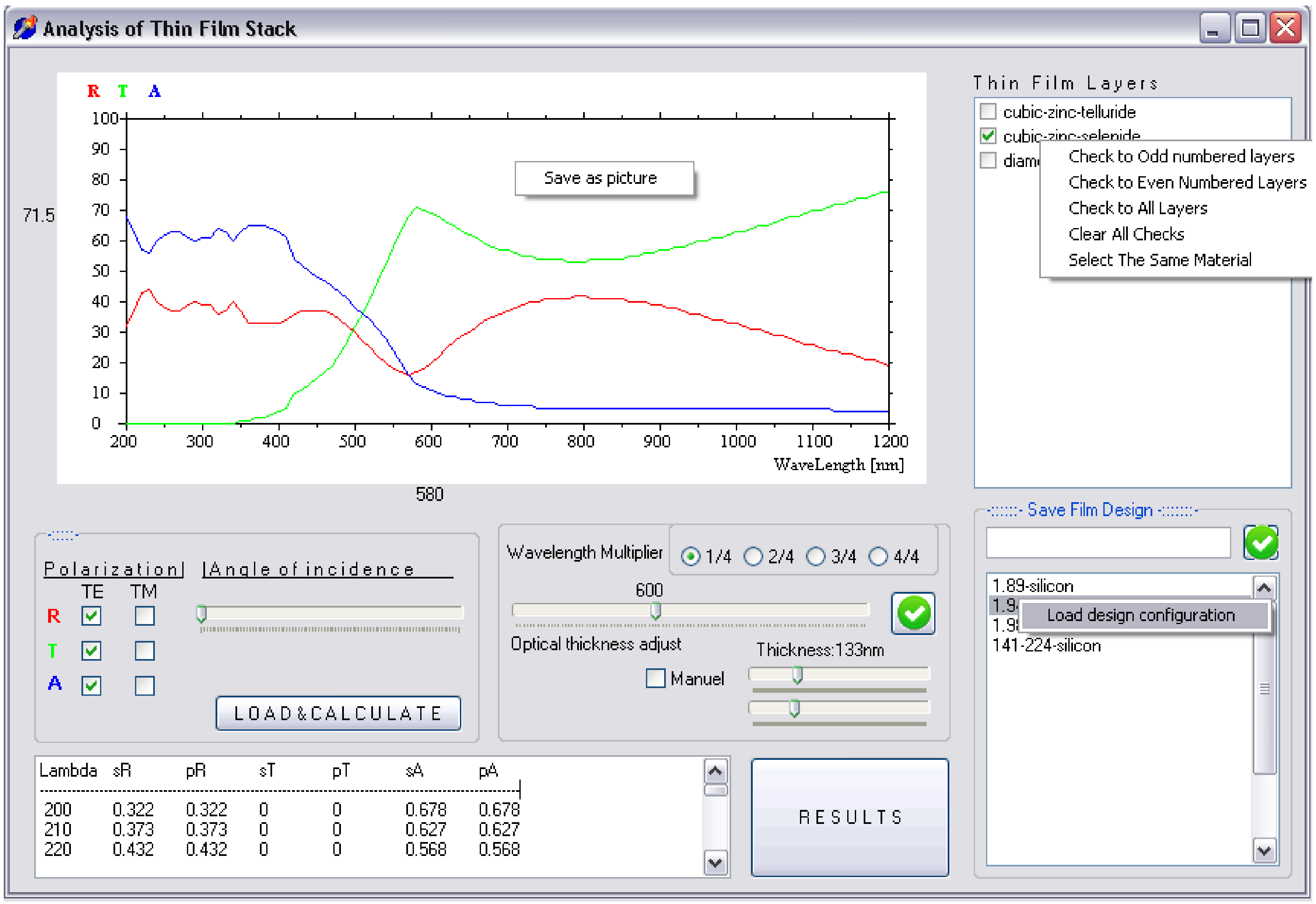


Figure 4.3: Print screen of the thin film stack design interface.

4.3 Simulation Interface

This simulation interface can be divided into five main parts as seen in Figure 4.4. Charting part is used for visualizing of calculation results. It has three different line colors. The red color is used for reflection, green color is used for transmission and blue color is used for absorbtion outputs. The vertical axis of the chart is scaled into 10 equal pieces having minimum 0 and maximum 100. The horizontal axis has minimum value 200nm and maximum value 1200nm.

At the left middle of the interface, thickness and incident angle input parameters are placed. This parameters can be changed practically by using trackbar components of delphi programming language. Thickness of the layers can be adjusted as their optical thicness multiplied with predefined multipliers ($\frac{1}{4}, \frac{2}{4}, \frac{3}{4}, \frac{4}{4}$). These multipliers are aimed for antireflection and high reflection conditions. $\frac{1}{4}$ and $\frac{3}{4}$ multipliers are used for antireflection and $\frac{2}{4}$ and $\frac{4}{4}$ multipliers are used for high reflection calculations. At the left bottom of the interface, all results can be taken as regular text for other programs.



☐ cubic-zinc-telluride
☑ cubic-zinc-selenide
☐ diam

R: TE ☑ TM ☐
T: TE ☑ TM ☐
A: TE ☑ TM ☐

Wavelength Multiplier: ● 1/4 ○ 2/4 ○ 3/4 ○ 4/4

Thickness:133nm

☐ Manuel

```
Lambda  sR     pR     sT   pT   sA     pA
200     0.322  0.322  0    0    0.678  0.678
210     0.373  0.373  0    0    0.627  0.627
220     0.432  0.432  0    0    0.568  0.568
```

1.89-silicon
1.9
1.9
141-224-silicon

Figure 4.4: Print screen of the analysis interface.

At the right side, used layers are listed in a listbox with checkbox in front of the layers. These checkboxes are used for selecting whether the layer should be infected or not with the thickness changes. This listbox has right click procedures which are used for checking the layers. If the checkbox of the layer is selected, then its thickness will be change instantly.

Right bottom of the interface is used for saving and loading configurations. When designed configuration is studied and decided to use later, then this configurations should be saved. At this step, graph is saved as bmp image file. Layer ordering and their thickness are appended to a memobox and all its lines are saved as text file under the settings folder. After saving procedure, all saved items are listed in a listbox.

By selecting the item in the listbox, bmp image file of that configuration is loaded to graph area immediatelly. when it is decided to study with their parameters, right click action should be used. At this step all configurations of layers, layer thickness and subrate parameters are loaded to interface in order to continue to advence study.

CHAPTER 5

PROGRAMMING ALGORITHMS FOR MATRIX CALCULATION

5.1 Functions of Matrix Calculation

An easy readable and understandable programming need good organized algorithms and all functions and procedures should be seperated. This provides simplicity and clarity while writing softwares. Functions use as many input parameters and they are returned to only single value assigned as Result. But procedures are different from functions. They can use input parameters as needed and produces many results.

All functions used for this program are classifed and all parameters belong to that function are showed in a table and written Delphi code is followed by its related table.

Tables contain inputs, output and explanations of used elements. Mathematical formulas of the related functions are placed into the top row of the all tables. Inputs are the elements used for the functions and output is the result of functions. Letters imply the variables used in the mathematical expressions. Explanation is used for the meaing of the that variable. Assigned value is the expressions that used in the coding environment and variable type tells us that parameter is double or complex or integer. Some times, some functions are used inside the other functions when they are needed. $\gamma = \sqrt{\frac{\varepsilon_0}{\mu_0}} = 0.002654$ is the admittance of the free space and it is used as a constant in the functions. Variables and formulas belong to simple function is organized as seen in Table 5.1 and Delphi code is written. Complete function tables and their codes are listed in appendix.

Table 5.1: Angle in terms of radians

$\theta = \pi \frac{angle}{180}$				
Inputs	Letter	Explanation	Variable	Variable type
	angle	Angle of incidence	angle	Double
Outputs	θ	Angle in terms of radian	Result	Double

```
Function teta(angle:Double):Double;
Begin
Result:=Pi*(angle/180);
End;
```

5.2 Procedures of Matrix Calculation

All data belong to materials are stored as text files seperately. When they are needed for processing, they are taken to memory and constants with respect to wavelength are placed into tree dimensional array. Dimensions of array are changed with respect to number of layers, but generally, wavelength numbers and n and k numbers are static, so one of the dimension is changeable as illustrated in Figure 5.1.

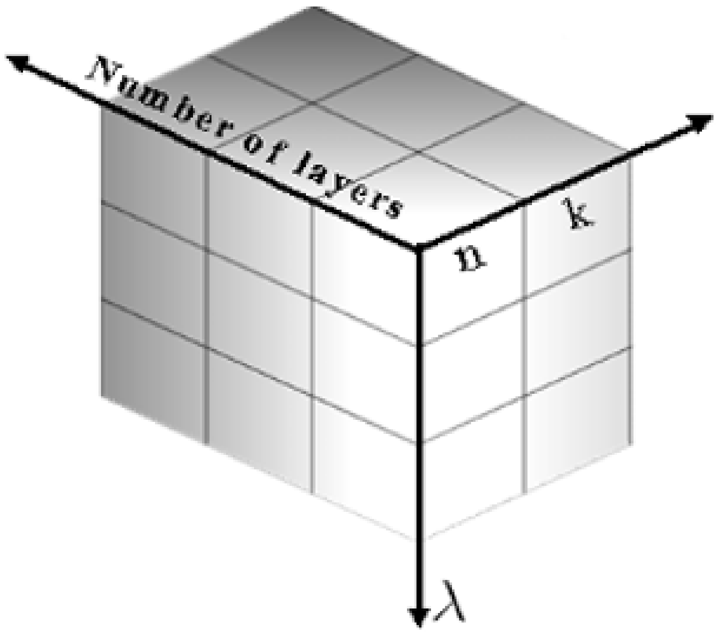
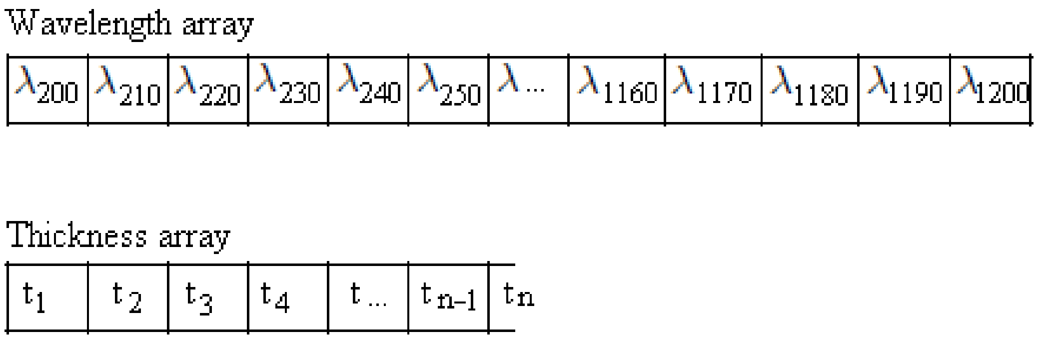


Figure 5.1: Storing optical constants of the materials in a 3D array.

Wavelength values and thickness of each layer are stored in a one dimensional array separately as shown in Figure 5.2.


Wavelength array

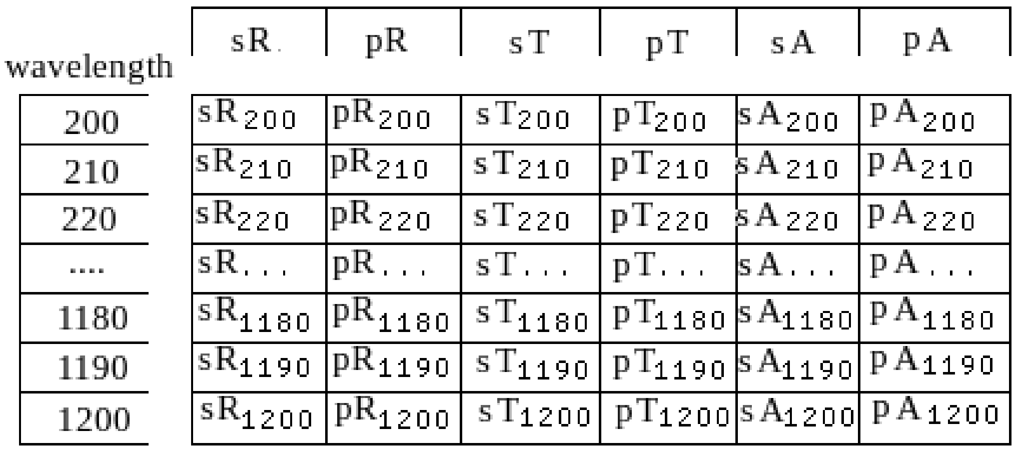
λ_{200}	λ_{210}	λ_{220}	λ_{230}	λ_{240}	λ_{250}	$\lambda_{...}$	λ_{1160}	λ_{1170}	λ_{1180}	λ_{1190}	λ_{1200}

Thickness array

t_1	t_2	t_3	t_4	$t_{...}$	t_{n-1}	t_n

Figure 5.2: One dimensional arrays for wavelength and thickness parameters.

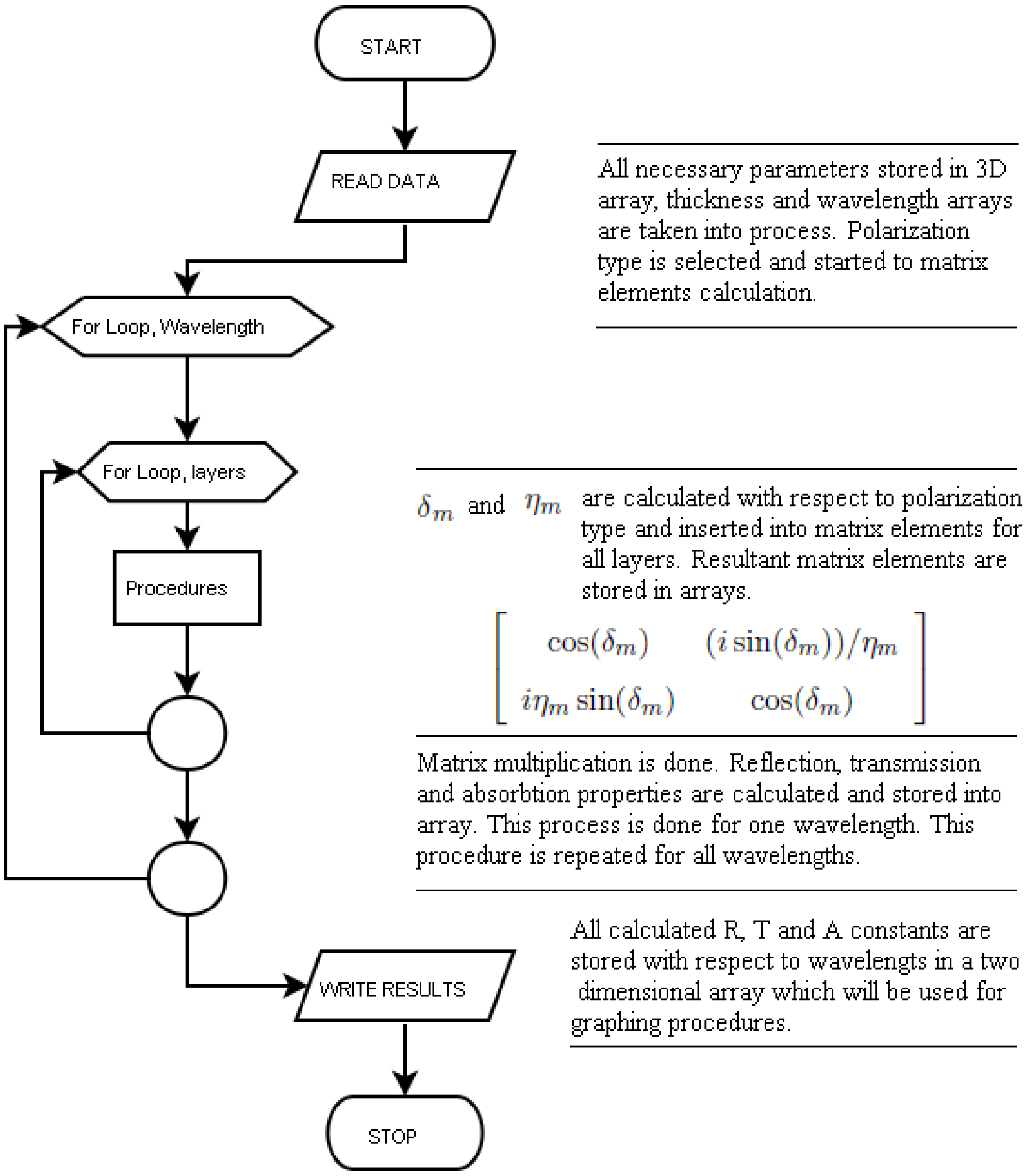
The core algorithm of the calculation is illustrated in Figure 5.4. All data belong to materials are stored in a three dimensional array. Reading and writing is done with arrays. Number of materials, wavelength range and complex refractive index ($N = n - ik$) are the main elements of dimensions of arrays. Refraction, transmission and absorption coefficients are obtained spectrally that is, inner loop is used for one wavelength and all procedures are repeated for all wavelength with the outer loop. And calculated results are stored in a two dimensional array in order to use it for graphing procedures as seen in Figure 5.3.



wavelength	sR	pR	sT	pT	sA	pA
200	sR_{200}	pR_{200}	sT_{200}	pT_{200}	sA_{200}	pA_{200}
210	sR_{210}	pR_{210}	sT_{210}	pT_{210}	sA_{210}	pA_{210}
220	sR_{220}	pR_{220}	sT_{220}	pT_{220}	sA_{220}	pA_{220}
....	sR. . .	pR. . .	sT. . .	pT. . .	sA. . .	pA. . .
1180	sR_{1180}	pR_{1180}	sT_{1180}	pT_{1180}	sA_{1180}	pA_{1180}
1190	sR_{1190}	pR_{1190}	sT_{1190}	pT_{1190}	sA_{1190}	pA_{1190}
1200	sR_{1200}	pR_{1200}	sT_{1200}	pT_{1200}	sA_{1200}	pA_{1200}

Figure 5.3: All calculated results are stored in a 2-dimensional array.

All procedures are repeated for the p-polarization and s-polarization with the same method. Due to difference in polarization, functions have changes but procedures are the same. This procedure is repeated for all wavelength values and these calculated results are stored in a two dimensional array with optical results corresponding to their wavelengths. Figure 5.4 is the flow diagram of the core program.



All necessary parameters stored in 3D array, thickness and wavelength arrays are taken into process. Polarization type is selected and started to matrix elements calculation.

δ_m and η_m are calculated with respect to polarization type and inserted into matrix elements for all layers. Resultant matrix elements are stored in arrays.

$$\begin{bmatrix} \cos(\delta_m) & (i\sin(\delta_m))/\eta_m \\ i\eta_m \sin(\delta_m) & \cos(\delta_m) \end{bmatrix}$$

Matrix multiplication is done. Reflection, transmission and absorbtion properties are calculated and stored into array. This process is done for one wavelength. This procedure is repeated for all wavelengths.

All calculated R, T and A constants are stored with respect to wavelengts in a two dimensional array which will be used for graphing procedures.

Figure 5.4: Flow diagram of the main calculation procedures.

For all layers, matrix elements must be calculated and placed into the arrays. Firstly δ_m and η_m calculation should be done and put into places in the matrix for a given wavelength. This step is pictured as Figure 5.5

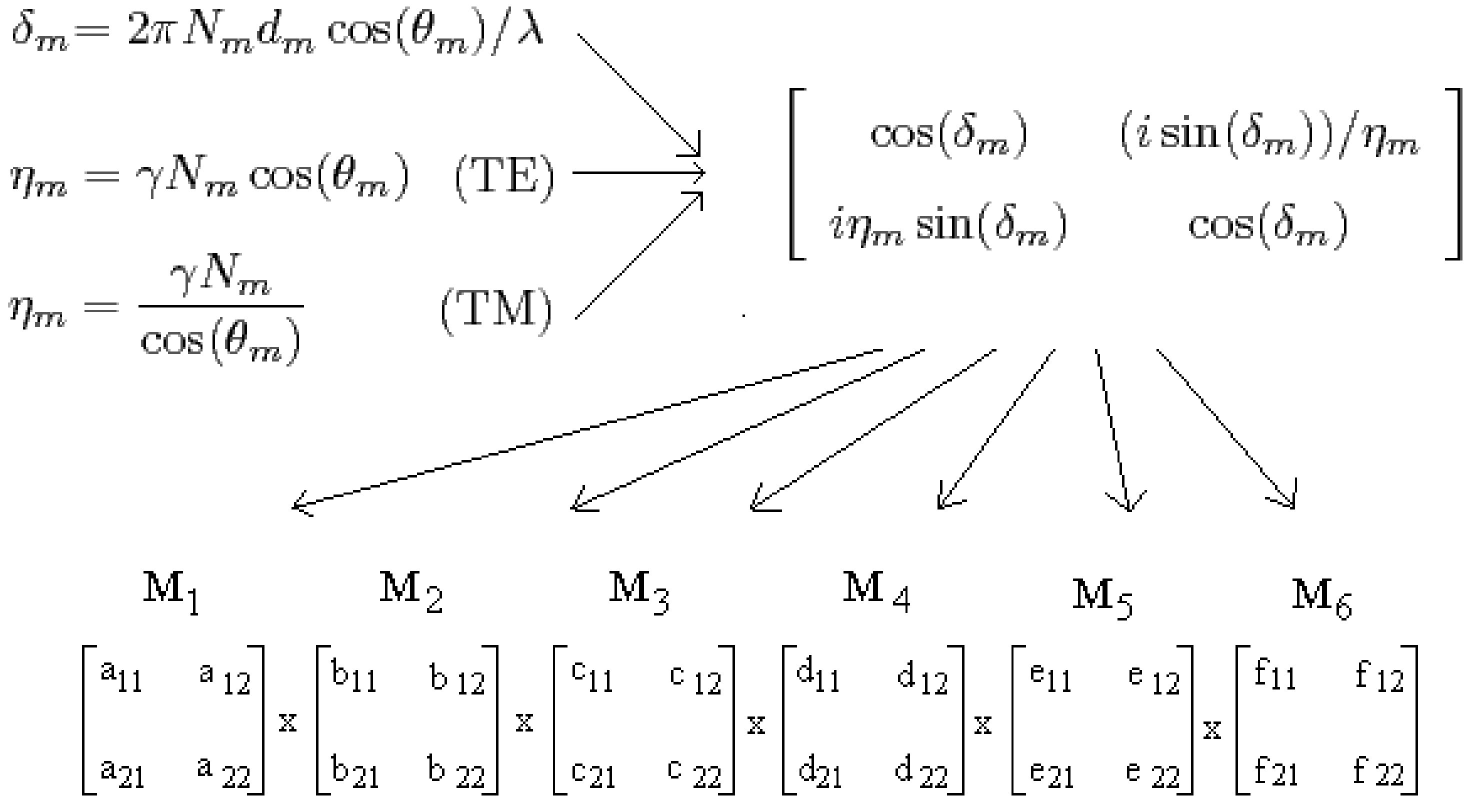


Figure 5.5: Filling the matrice elements.

In order to make matrix multiplication over an array, extra two matrix are used as temporarily. M_R matrix is unit matrix at the beginning and it is multiplied with first matrix and results are placed into temporary matrix M_t after completing first multiplication, M_t is moved to M_R and new M_R matrix is multiplied with second matrix and results are collected again M_t matrix, after second multiplication M_t is moved to M_R matrix and this procedure is repeated until last matrix element is multiplied. This procedure is illustrated in Figure 5.6. By using this practical multiplication method, huge number of matrix elements are multiplied easily.

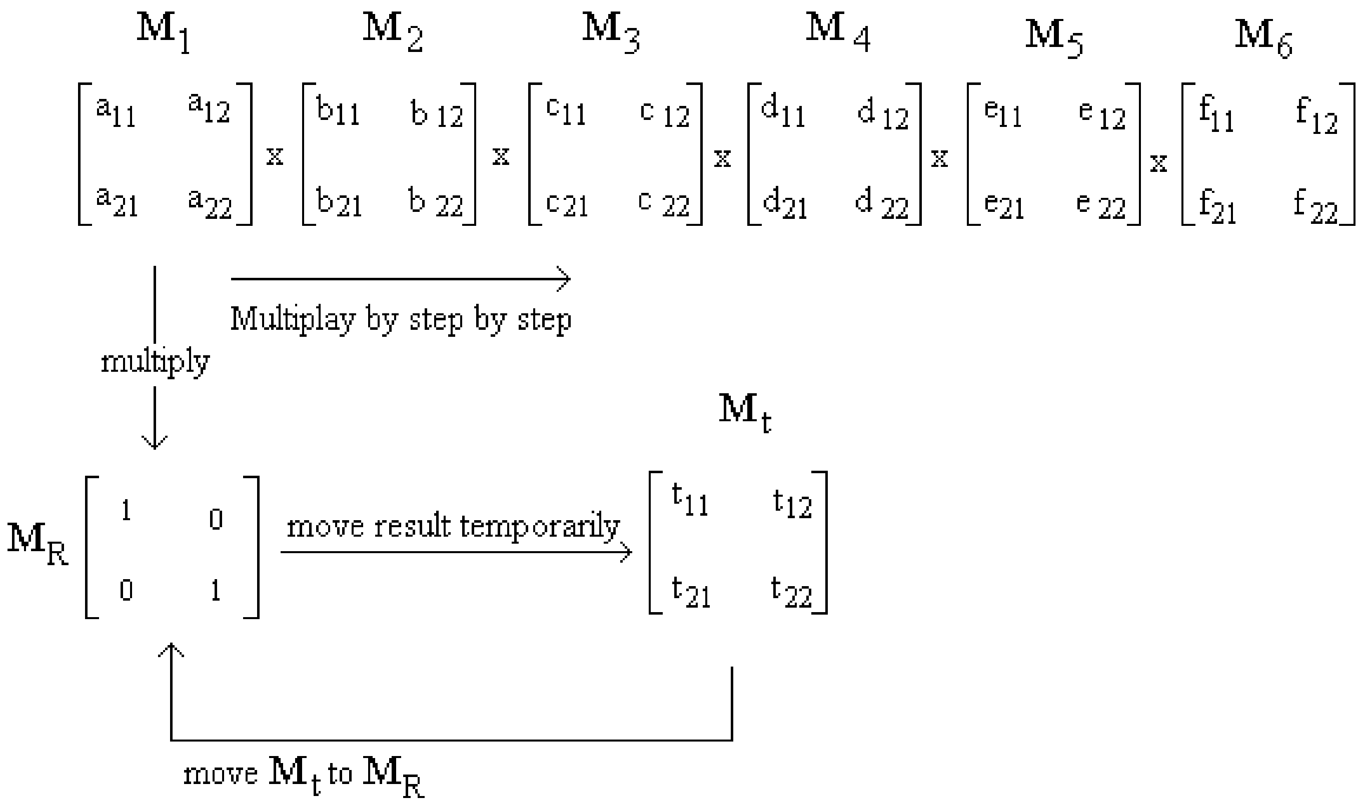


Figure 5.6: Multiplication of the matrix elements.

After matrix multiplication is obtained, the next calculations are *B* and *C* values. This is done by multiplication of resultant matrix with matrix element belong to substrate parameters. These obtained *B* and *C* values are used for the resultant optical parameters, reflectance, transmittance and absorbtance.

Displaying calculation resulst are very straight forward. All results are recalculated in order to fit for a scaled region. Delphi has great opportunity about canvas procedures. First of all, results are taken from the array and recalculated in order to make fit to the limited region and it is assigned on the image area. For the following wavelength the same method is applied and assigned on the image area. These two assigned points are connected with a straight line. Mainly two Delphi procedures, Canvas.MoveTo and Canvas.LineTo, are used for assigning points and connecting two points with a line. Flow diagram and basic picture of produced are shown in Figure 5.7. Complete Delphi code is given in appendix.

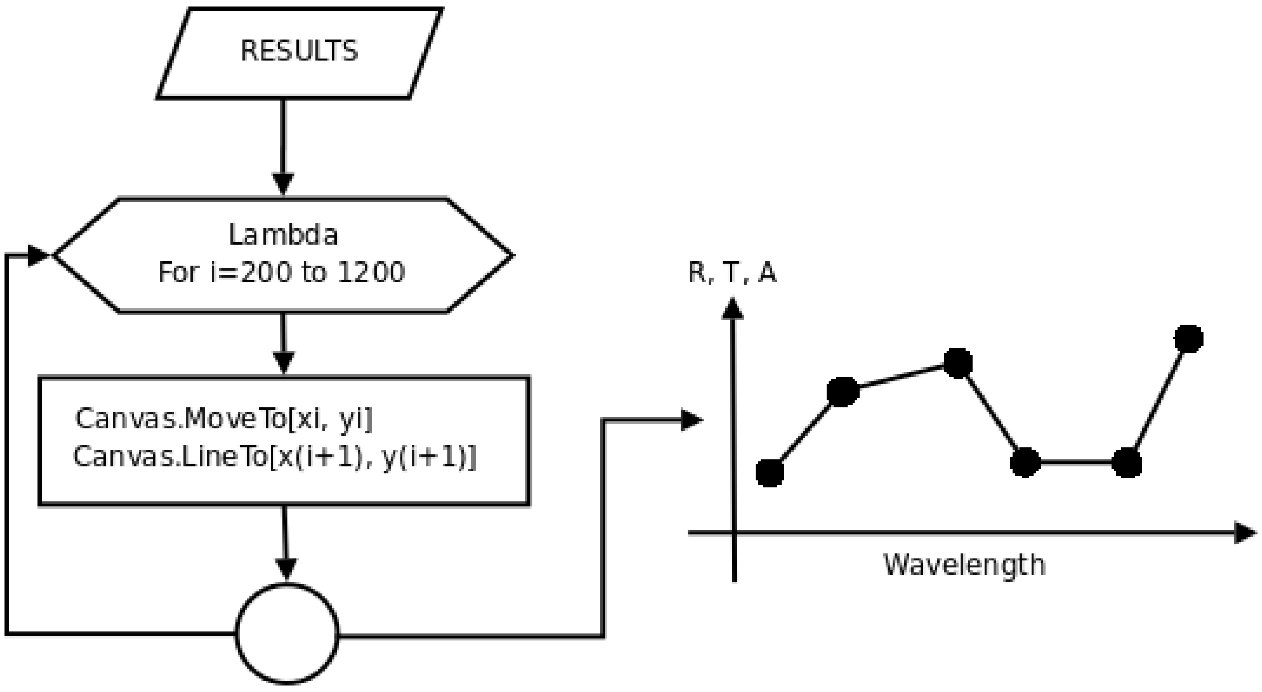


Figure 5.7: Procedure flow diagram and sssigned points and connection lines on graph.

The distance between two points is so small that, smooth continuous curves are obtained. This dual point connection is repeated until the last wavelength values are assigned. Axis and scales on the chart are manually constructed. And all axis length and other variables are defined as constants in the procedure. These constants are used for chart width, height, scaler and label positions. An example of this type of chart produced is pictured as Figure 5.8.

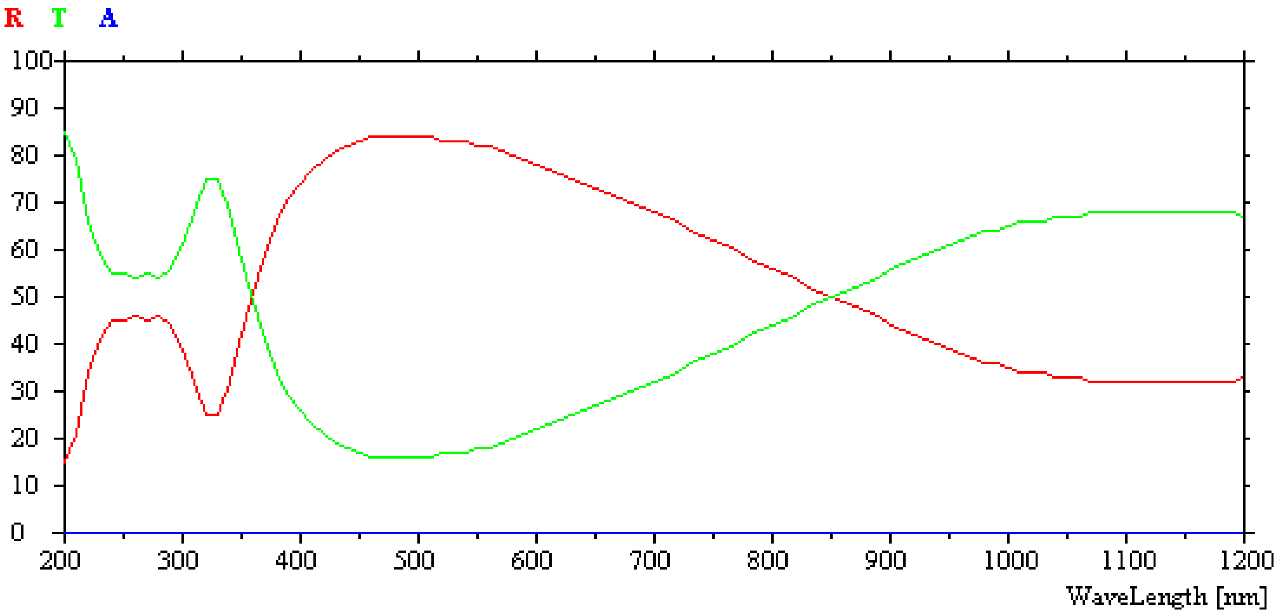


Figure 5.8: An example chart

CHAPTER 6

TEST OF THE PROGRAM OUTPUTS WITH STUDIED MATERIALS

Designed software needs comparions with the examples of the studied articals. This makes it more reliable. Studied examples include both the theoretical calculations and experimental results. The optical constants of the materials in the scientific papers are used in the software comparatively.

6.1 Single Layer Antireflective Coating Examples

The simplest form of anti-reflection is a single layer deposited on a surface. In order to get anti-reflection, this single layer should have cancellation of light at the upper and lower surface of its two surfaces. Assume that outer medium (air) has refractive index n_0, that of coating thin film is n_1 and the substrate is n_2. Then, in order cancel the two reflected beams, the intensities of radiation reflected at upper and lower boundaries should be equal, that is: ratios of the refractive indices at each boundary should be equal.

$$\frac{n_0}{n_1} = \frac{n_1}{n_2} \tag{6.1}$$

or

$$n_1 = \sqrt{n_0 n_2} \tag{6.2}$$

Also, coating should produce destructive interferences between the beams reflected from the front face of the film and back face of the film. This achieved if both reflections at interfaces from the first medium and the following medium have 180^o phase differences. Snell's Law is $n_0\lambda_0 = n_1\lambda_1 = n_2\lambda_2$, $n_0 = 1$, therefore layer thickness should be $d = \frac{\lambda_0}{4n_2} = \frac{\lambda_2}{4}$. Thus, a simple single anti-reflection layer should have a refractive index equal to the square root of that of the substrate, and should be one quarter of wavelength of optical thickness [10]. In the Figure 6.1, single layer anti reflection candidate is calculated.

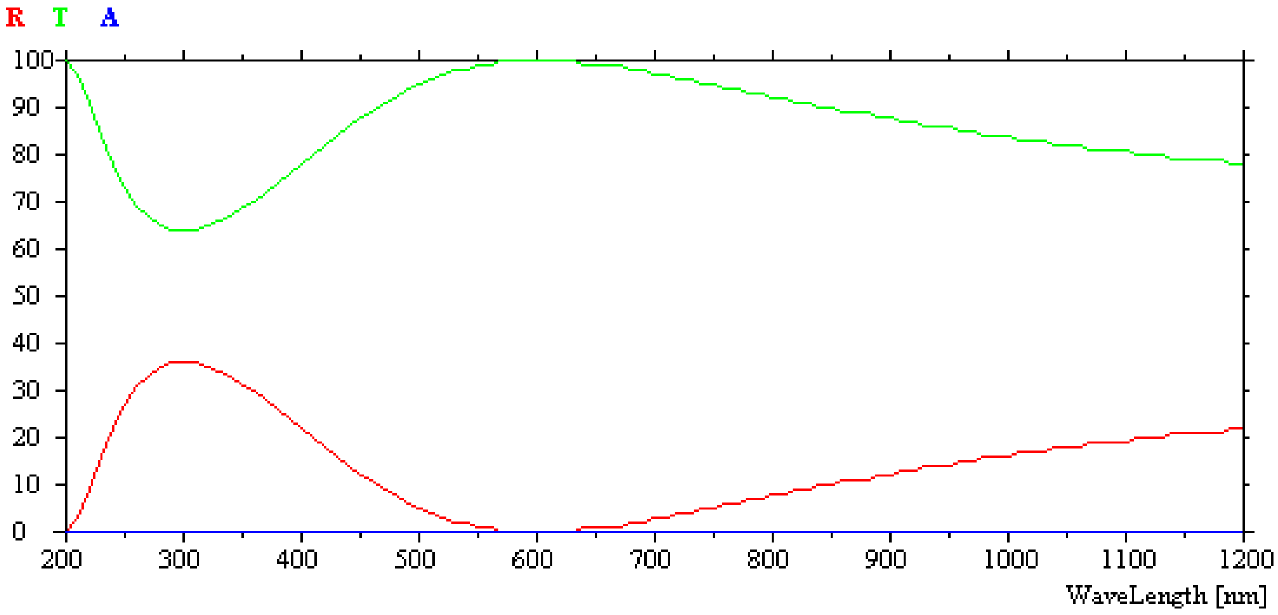


Figure 6.1: Single layer anti-reflective calculation. Substrate refractive indice is $n_s = 4$ and film layer has $n_1 = 2$ and outer medium is air. Film thickness is 75nm.

Silicon is used as a substrate commonly. Its refractive indices are optained from HOC and imported to our software and its optical constants are showed in Figure 6.2.

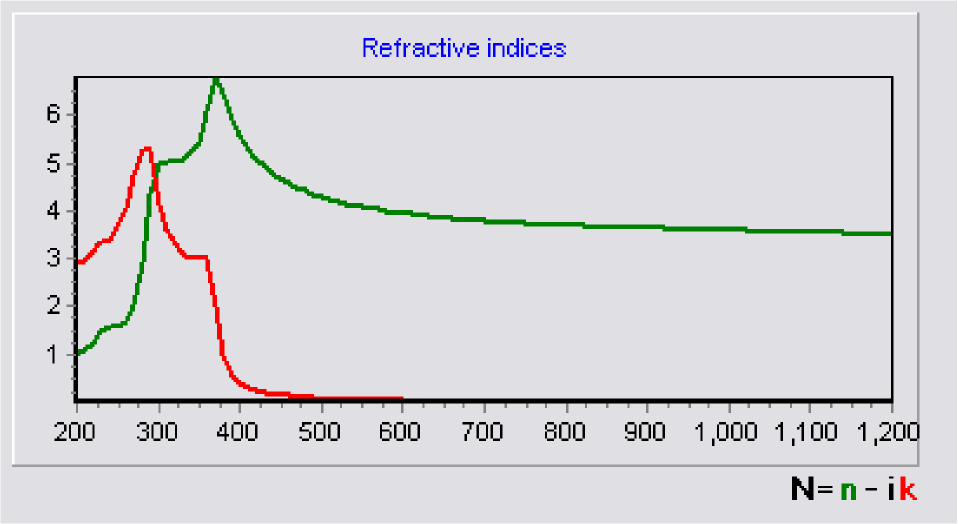


Figure 6.2: Refractive indices of the silicon with respect to wavelength.

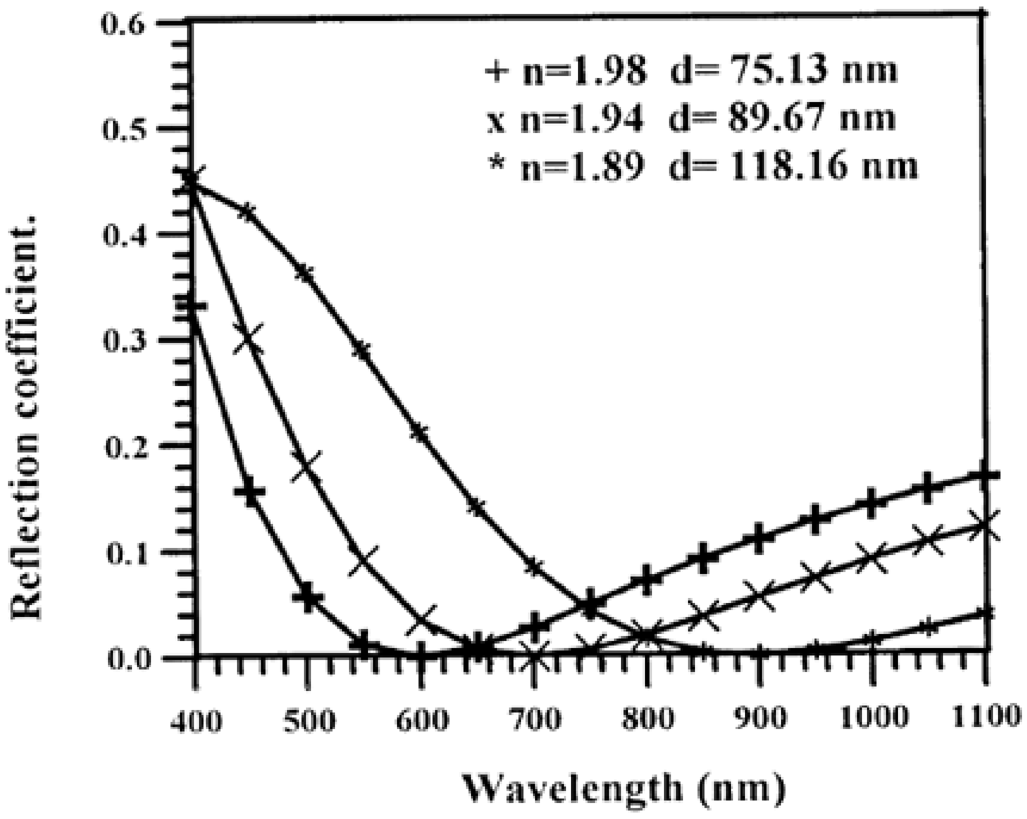


Figure 6.3: Reflectance spectra vs. wavelength for some optimised single-layer antireflection coating on silicon substrate [11].

In this study, the reflectance spectra of three optimised single-layer antireflective systems are optimized with their refractive indices and film thickness. In this calculation, $n = 1.98$, $n = 1.94$ and $n = 1.89$ values are constant for all wavelengths. But refractive indice for silicon is not constant and it shows variety as seen in Figure 6.2. Green line is used for real part of the index and red line is used for complex value of the refractive indices. Parameters in Figure 6.2 are used in the designed software and all three results are showed in Figure 6.4. In this software, thickness valuse are integer type and so the above thickness parameters in Figure 6.3 are rounded.

In Figure 6.4, all the outputs of the software are well compatible with the results showed in Figure 6.3. This is the experience for the single layer coatings. So we can calculate reflectance, transmittance and absorbtance for any single layer coated on a substrate easily. For more reliability, this procedure should be repeaded for double layer and multi layers as possible as.

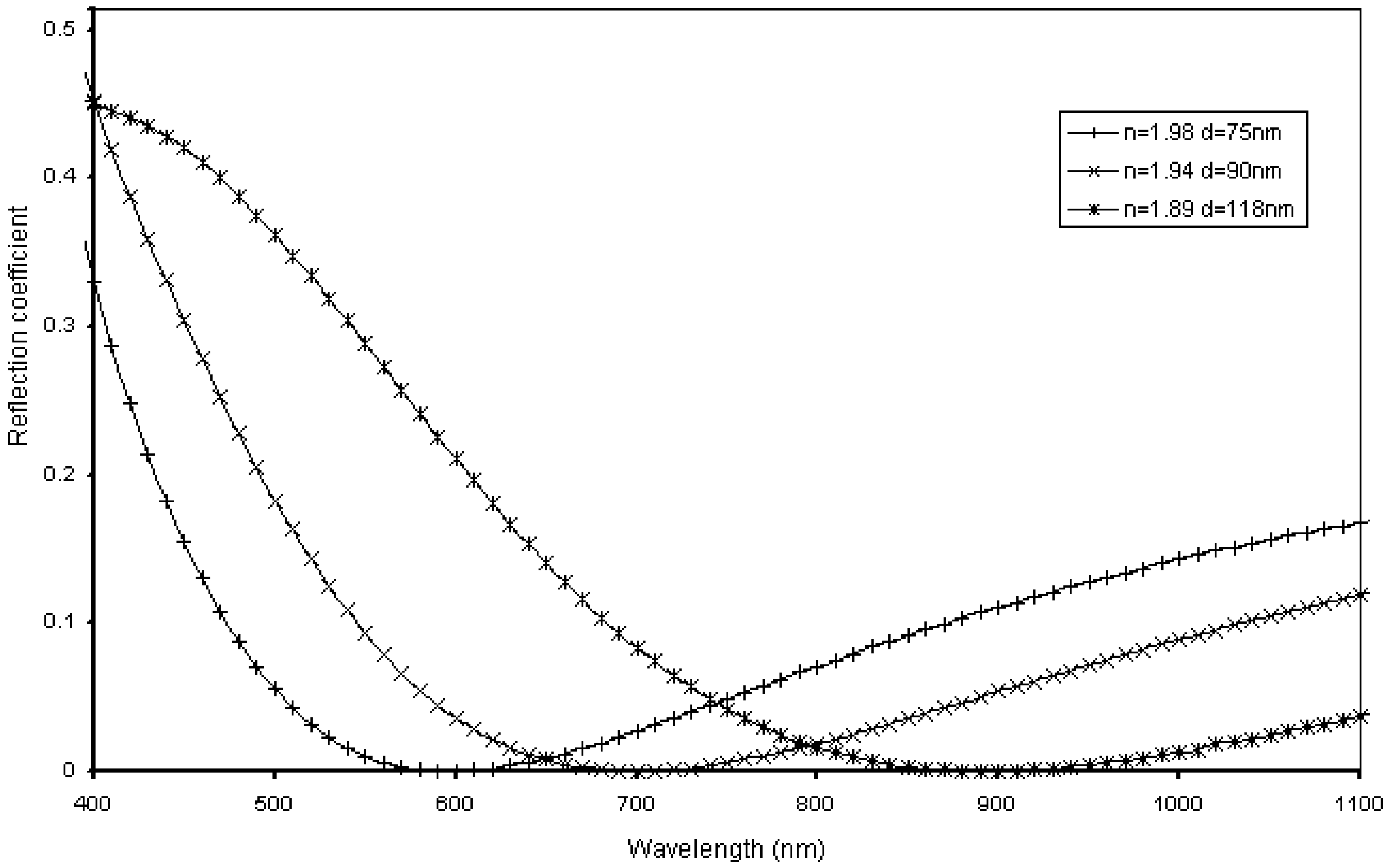


Figure 6.4: Reflectance spectra vs. wavelength for three single-layer coatings seperately over silicon substrate with their thicknesses.

6.2 Two-layer antireflective coating designs

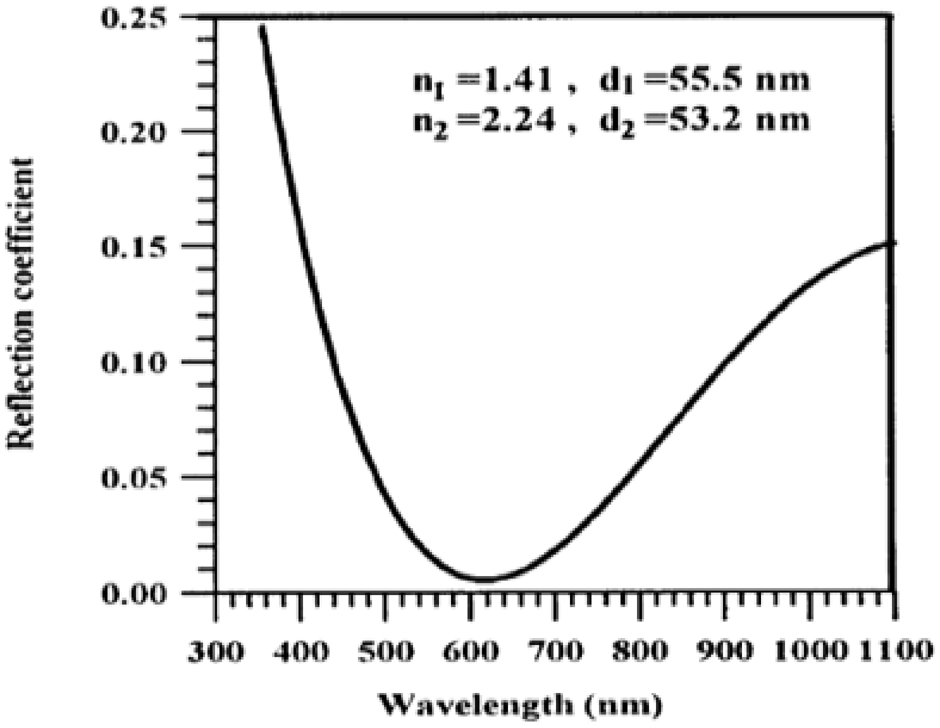


Figure 6.5: Reflectance spectra vs. wavelength for double-layer antireflection coating on silicon substrate [11].

The parameters are applied to the software and results are showed in Figure 6.6. In this software all graphics have the same scaler and size. Due to this situation, the pictures taken from the articles and the images of the software have difference in terms of scaler and appearance. But as we can consider about the values on the curve, they are compatible with each others.

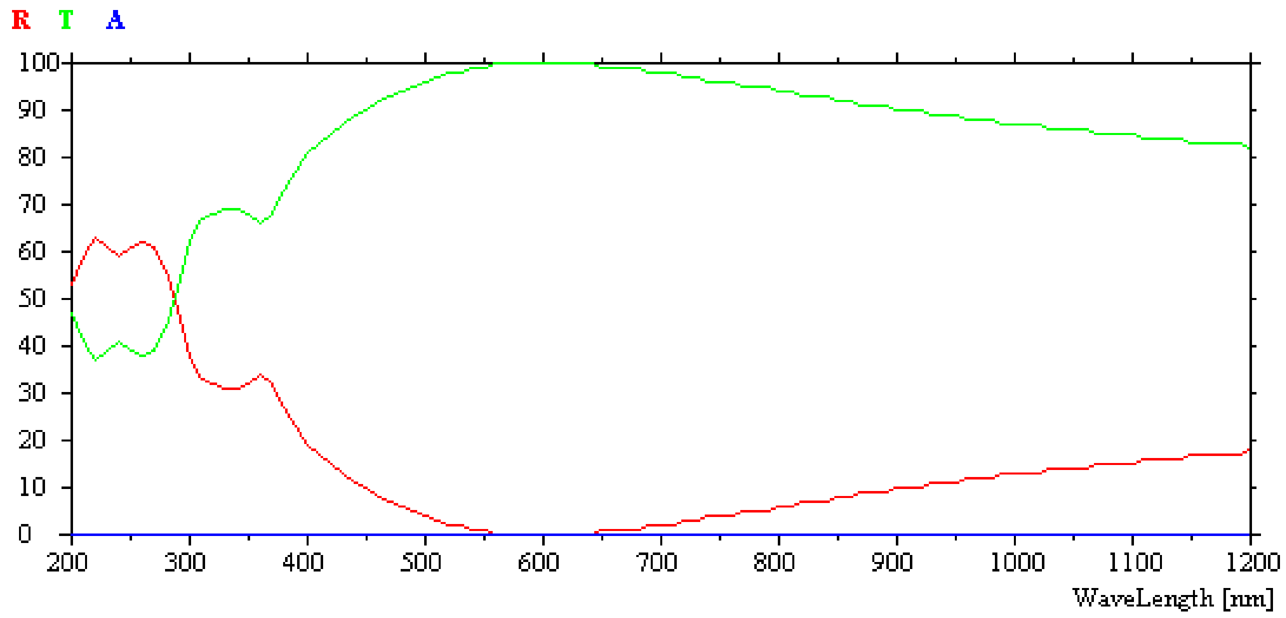


Figure 6.6: Double-layer antireflection coating on silicon substrate with values n_1 = 1.41 and n_2 = 2.24, thickness parameters are 56nm and 53nm.

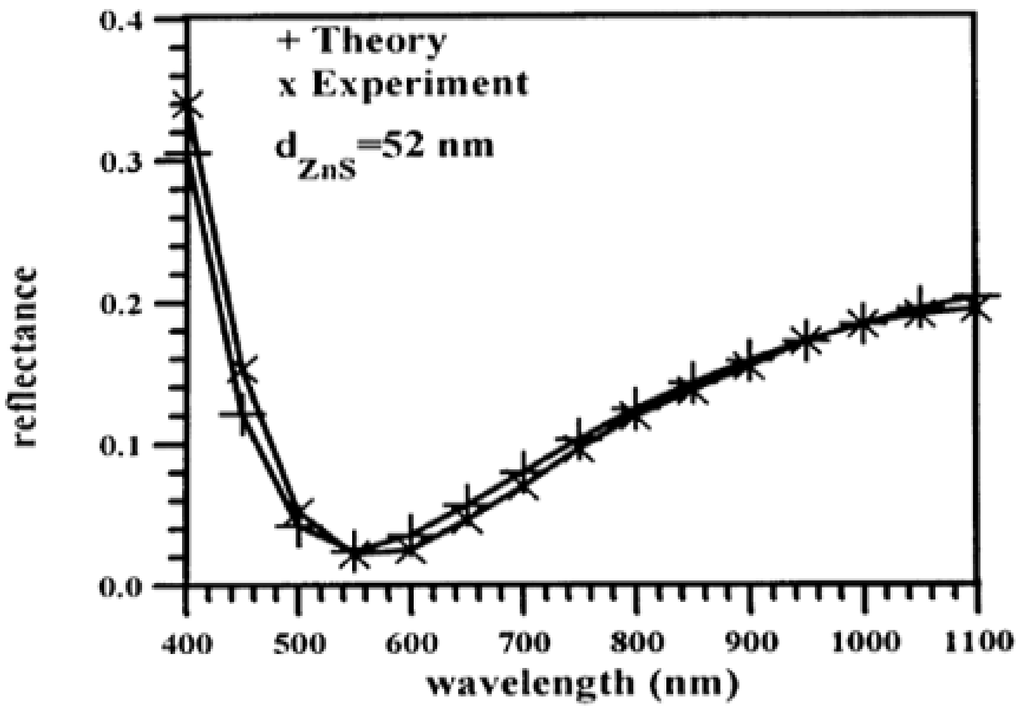


Figure 6.7: Measured and calculated spectral reflectance of ZnS antireflective coating on silicon [11].

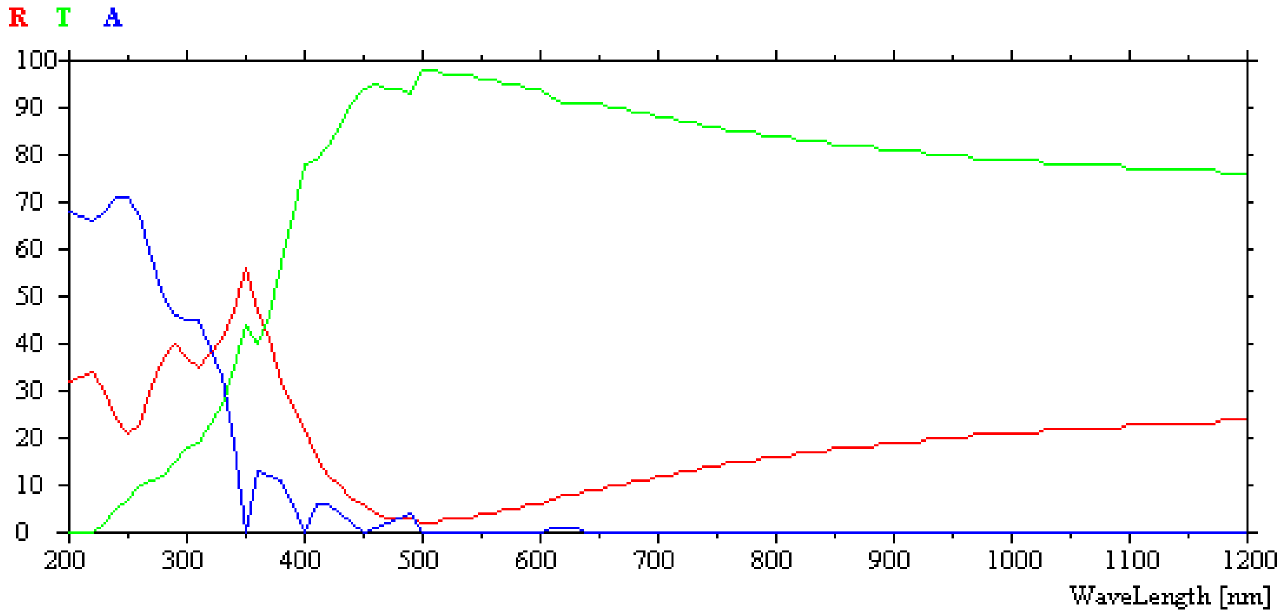


Figure 6.8: Calculated spectral reflectance of ZnS antireflective coating on silicon.

In this example there is a little shift towards to the left. This may be result of the differences between two optical indices used in the article and in our software. ZnS material used in our software has cubic structure so this may be cause of the differences. Refractive indices spectra of the cubic ZnS are shown in Figure 6.9.

Figure 6.9: Refractive indices of the cubic ZnS.

6.3 Multi layer application exapmles

Multilayer study has more parameters and results are more affected by these parameters. So calculation errors will be more than one or two layer coatings results. In this example AlN and GaN materials are coated on sapphire substrate. AlN/GaN bilayers are repeated 25 times and total layer count is 50. AlN, GaN and sapphire have refractive index at $\lambda = 467nm$, $n_{AlN} = 2.16$, $n_{GaN} = 2.44$ and $n_{sapphire} = 1.78$, recpectivelly. The thickness measured for AlN and GaN were 62.3 and 40.3 nm, respectively [12]. Result is shown in Figure 6.10.

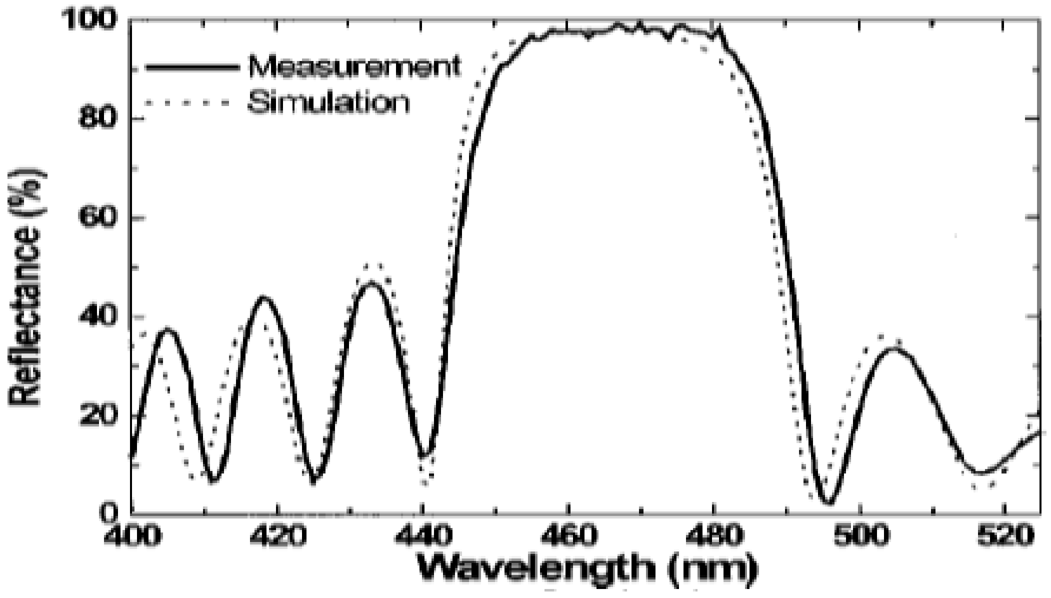


Figure 6.10: Measured and simulated reflectance spectra of the $(AlN/GaN)^{25}$ on sapphire substrate [12].

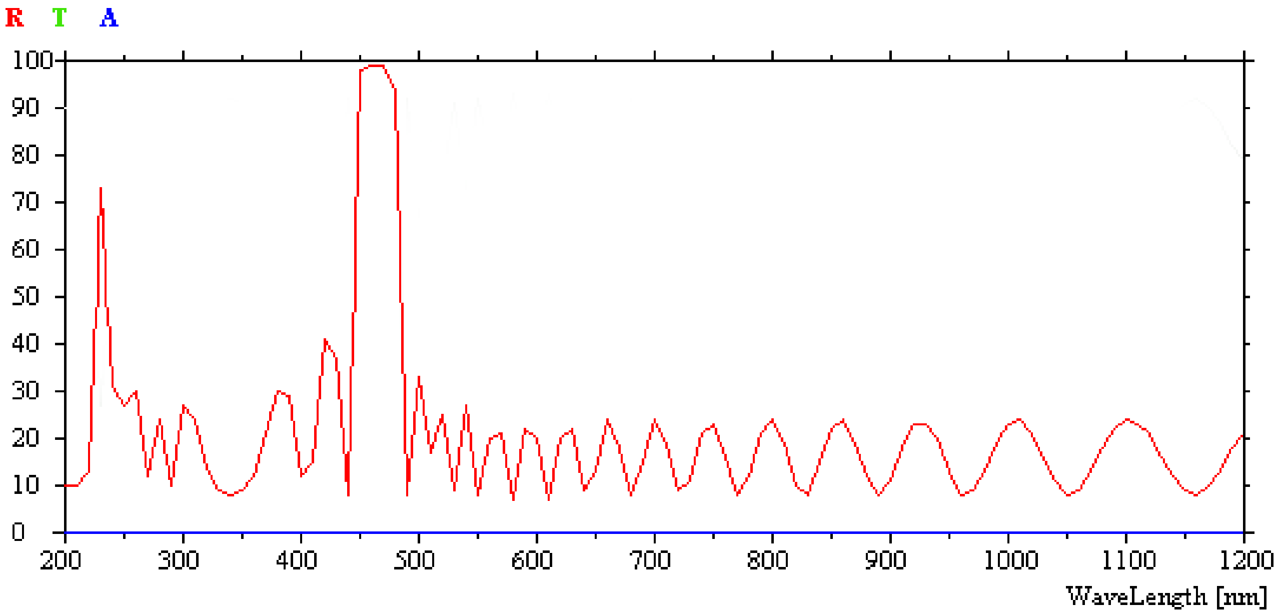


Figure 6.11: Simulated reflectance spectra of the $(AlN/GaN)^{25}$ on sapphire substrate. Thicknesses are AlN 62nm, GaN 40nm.

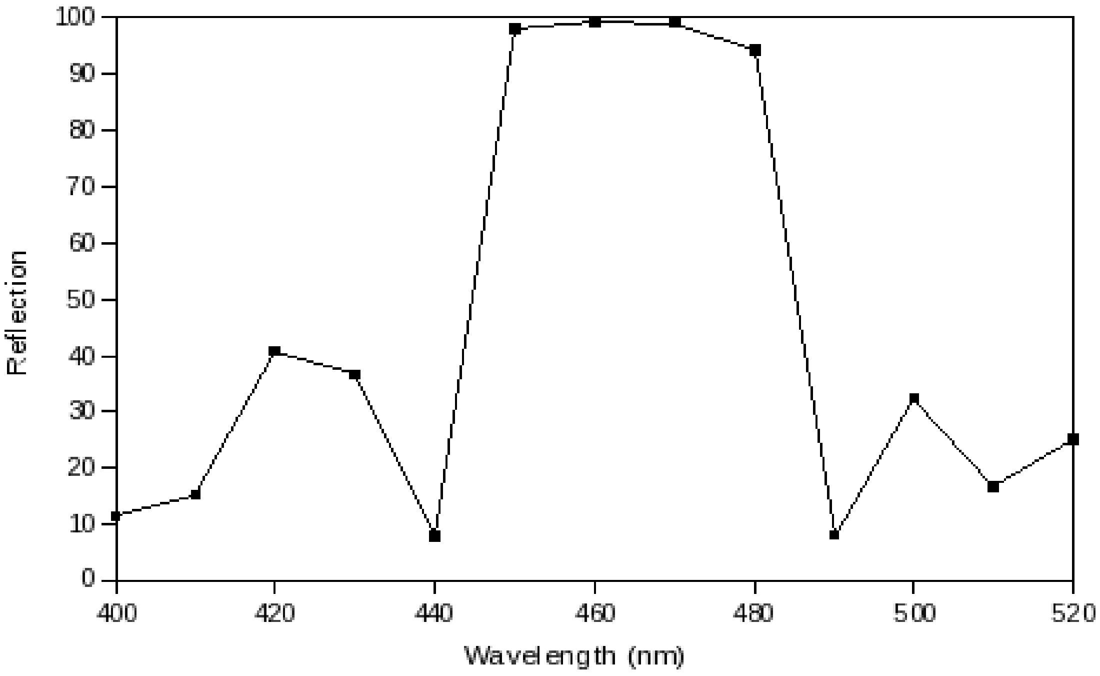


Figure 6.12: Simulated reflectance spectra of the $(AlN/GaN)^{25}$ on sapphire substrate.

Figure 6.11 is redrawed as rescaled in Excell program. In Figure 6.10 GaN refractive index data is used spectrally. But in Figure 6.11 and Figure 6.12 GaN refractive index is taken as constant for all wavelength. Because data is not available in the our program. So, results have difference except in the regions of $\lambda = 467nm$. As seen in this example, our program produces a valid result competible with the experimental and theoretical studied materials.

Program is also tested with the same material having different thickness and layer numbers. For example, single layer having thickness 400nm is simulated and results are saved. Then, this single layer is divided into 100 pieces and layers having 4nm thickness each. Aboslutely, there is no any physical changes. Both designs are the same but many layer numbers mean many matrix items. All simulations with different configurations have the same results. These experiences verify that, matrix calculations work fine. Also this kind of test is applied with different incident angles and the same results are obtained. So there is not any problem with different incident angles. Consequently by trusting these tests, different kind of multilayer designs such as antireflective coatings, high reflective mirrors and spectral optical filter designs can be done.

CHAPTER 7

CONCLUSION

So far, characteristic matrix method and optical properties of thin films are studied and a computer program has developed for difficult and tremendous calculation. In order to calculate reflection, transmission and absorption of a thin film stack, index of refraction with complex value and thickness of the each films are necessary inputs of the computer program.

Refractive index is material dependent and playing on this parameter is not possible, the only variable input parameter is the thickness of the film. But, finding candidate index of refraction may be obtained by selecting from the most adjacent materials. This is difficult because all index of refraction values are wavelength dependent and may have valuable differences spectrally. On the contrary, thickness of the film is arbitrary parameter and it can be adjusted from several nanometer to micrometer.

Developed computer program is tested with the studied materials and calculation results are compatible with the theoretical and experimental ones. Results have a little differences in some examples. Because, refractive index parameters are taken as a constant spectrally. But calculations about reference wavelength (wavelength whose refractive index is used as constant for all wavelength) are well compatible. On the contrary, there will be considerable changes far away from the reference wavelength. In order to get better results, complex refractive indices of each materials should be used spectrally.

Computer software technology is indispensable for complicated and involved calculations in our today thin film technology. This kind of thin film design is not possible without this technology. Once basic software is developed for this type of involved calculations, this meaningful study can be developed for more complicated and extended thin film design.

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Appendices

Appendix A

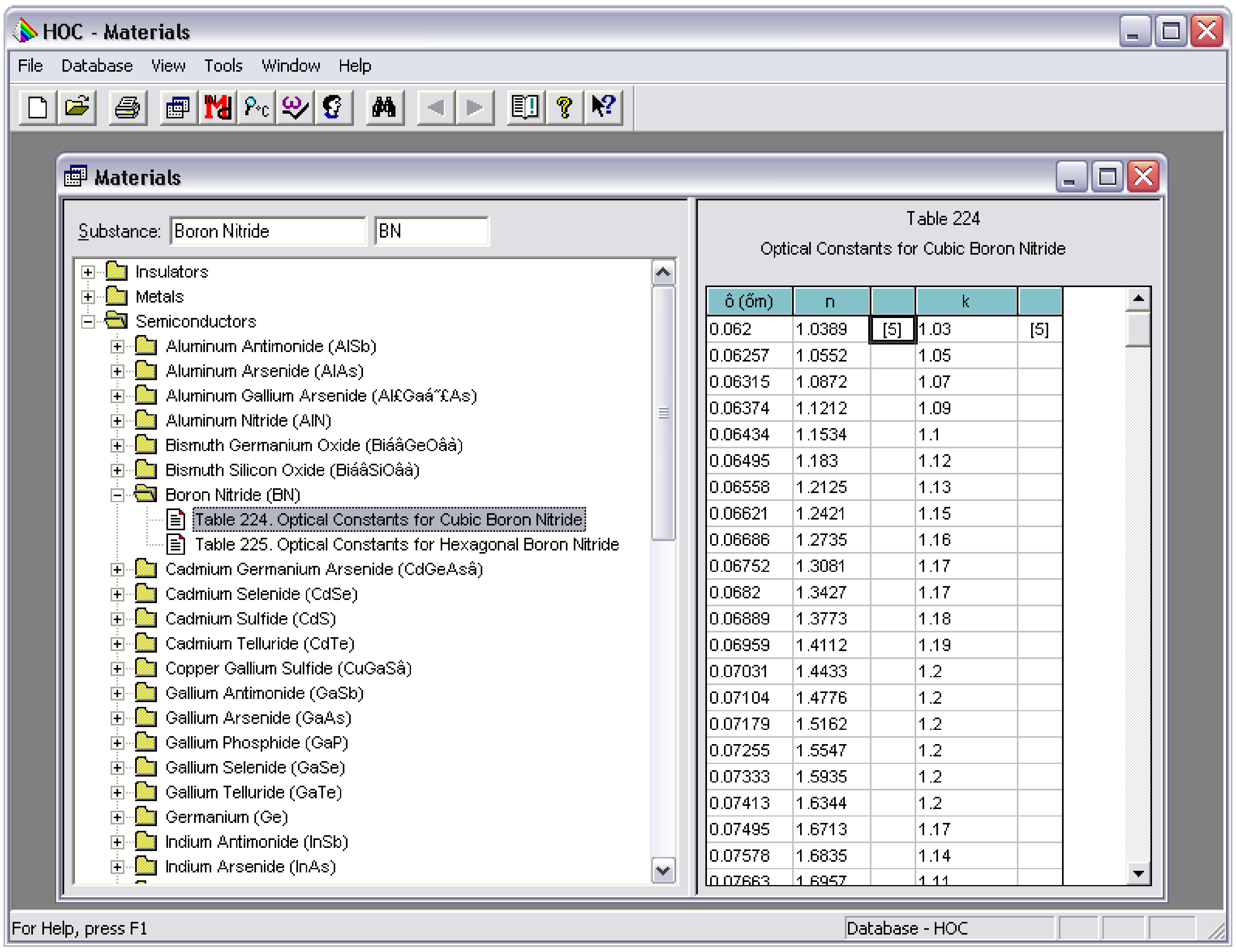
HANDBOOK OF OPTICAL CONSTANTS OF SOLIDS (HOC)

A.1 Introduction to Software

The HOC includes the optical constants prepared as electronically from the 5 volume set of hardcopy of Handbook of Optical Constants. HOC gives optical constants in a dynamic data table, displays constants in 2D or 3D graph and makes property calculations.

The program is designed for material scientists, spectroscopists, and optical device designers who work with dielectric materials, including metals, semiconductors, and insulators. The main HOC database includes both the data on optical constants and the Critiques written by world-known specialists; the data, the methods used to obtain them, and the validity of the information are thoroughly discussed there.

A.2 User Interface and the Functionalities of the HOC Software



Substance: Boron Nitride BN

- Insulators
- Metals
- Semiconductors
  - Aluminum Antimonide (AlSb)
  - Aluminum Arsenide (AlAs)
  - Aluminum Gallium Arsenide (Al£Gaá˜£As)
  - Aluminum Nitride (AlN)
  - Bismuth Germanium Oxide (BiáâGeOâà)
  - Bismuth Silicon Oxide (BiáâSiOâà)
  - Boron Nitride (BN)
    - Table 224. Optical Constants for Cubic Boron Nitride
    - Table 225. Optical Constants for Hexagonal Boron Nitride
  - Cadmium Germanium Arsenide (CdGeAsâ)
  - Cadmium Selenide (CdSe)
  - Cadmium Sulfide (CdS)
  - Cadmium Telluride (CdTe)
  - Copper Gallium Sulfide (CuGaSâ)
  - Gallium Antimonide (GaSb)
  - Gallium Arsenide (GaAs)
  - Gallium Phosphide (GaP)
  - Gallium Selenide (GaSe)
  - Gallium Telluride (GaTe)
  - Germanium (Ge)
  - Indium Antimonide (InSb)
  - Indium Arsenide (InAs)

Table 224

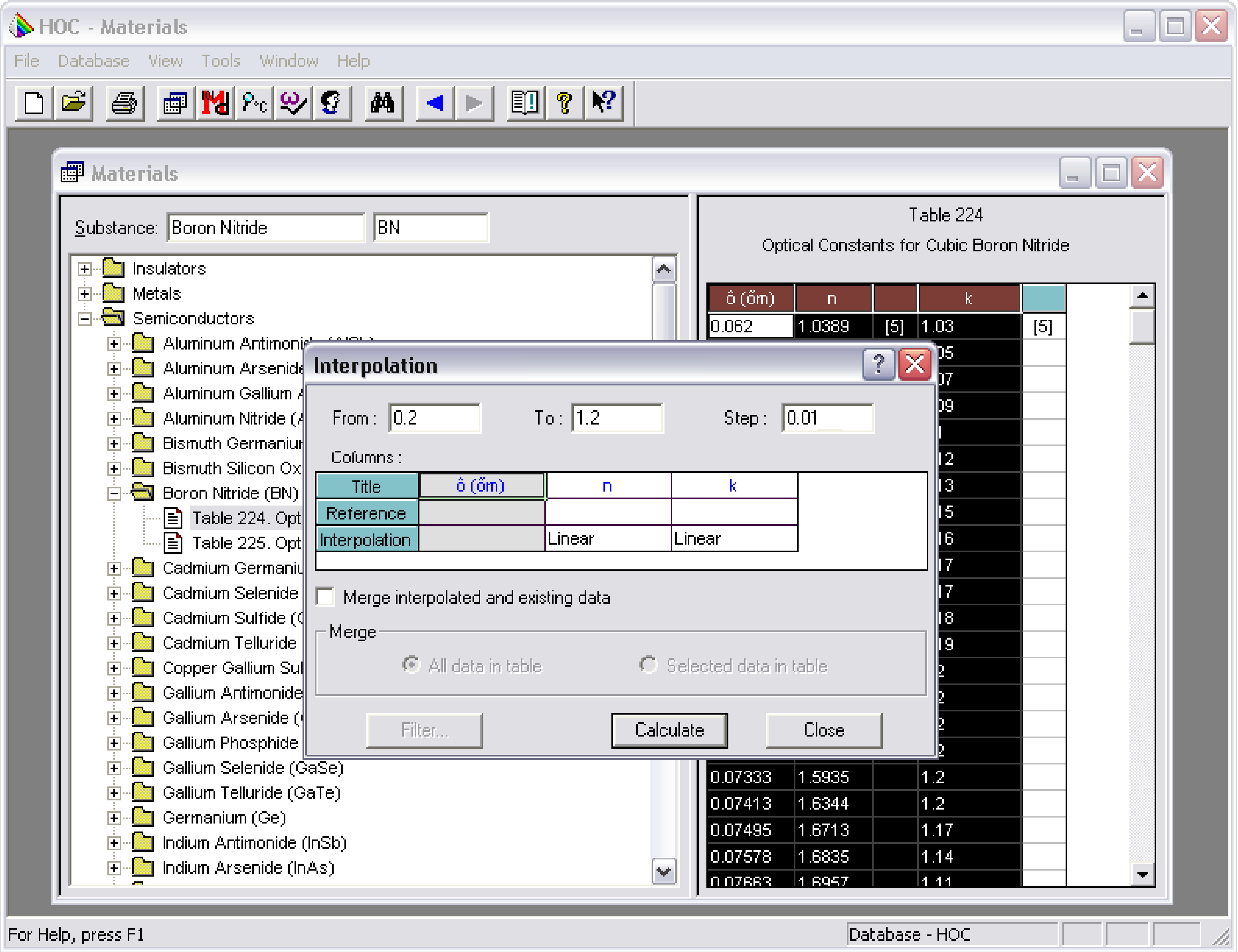
Optical Constants for Cubic Boron Nitride

ô (õm)	n		k	
0.062	1.0389	[5]	1.03	[5]
0.06257	1.0552		1.05	
0.06315	1.0872		1.07	
0.06374	1.1212		1.09	
0.06434	1.1534		1.1	
0.06495	1.183		1.12	
0.06558	1.2125		1.13	
0.06621	1.2421		1.15	
0.06686	1.2735		1.16	
0.06752	1.3081		1.17	
0.0682	1.3427		1.17	
0.06889	1.3773		1.18	
0.06959	1.4112		1.19	
0.07031	1.4433		1.2	
0.07104	1.4776		1.2	
0.07179	1.5162		1.2	
0.07255	1.5547		1.2	
0.07333	1.5935		1.2	
0.07413	1.6344		1.2	
0.07495	1.6713		1.17	
0.07578	1.6835		1.14	
0.07663	1.6957		1.11	

Figure A.1: Material tree view of the HOC software.

The Materials tree interface provides all optical data and information in the form of dynamic data table on a selected material. Materials are classified as insulators, metals and semiconductors. Refractive index, extinction coefficients, Sellmeier coefficients and Thermo-Optical Coefficients are obtained for 143 key materials. In this thesis study only refractive index and extinction coefficients with respect to wavelength are interested. Data on the dynamic table can be interpolated with desired variables. This provide a more appropriate and classified data to the other applications.

This software provides convenience about finding materials by using periodic table. When desired material is selected from the periodic table, this interface finds the materials and its components through 143 key materials. As seen Figure A.1 material trees and optical coefficients belong to selected material are displayed.



Substance: Boron Nitride BN

Table 224

Optical Constants for Cubic Boron Nitride

ô (őm)	n		k	
0.062	1.0389	[5]	1.03	[5]
0.07333	1.5935		1.2	
0.07413	1.6344		1.2	
0.07495	1.6713		1.17	
0.07578	1.6835		1.14	
0.07663	1.6957		1.11	

From : 0.2 To : 1.2 Step : 0.01

Title	ô (őm)	n	k
Reference			
Interpolation		Linear	Linear

☐ Merge interpolated and existing data

Figure A.2: Interpolation interface of the HOC software.

The optical parameters belong to materials have changes from material to material. So the best way of overcoming this problem, all parameter of the materials are interpolated with the same starting and ending point and with the same wavelength interval. As seen in Figure A.2, linear interpolation is done from 0.2μm to 1.2μm with a step value 0.01μm.

Appendix B

FUNCTIONS OF MATRIX CALCULATION

Table B.1: Angle in terms of radians

$$\theta = \pi \frac{angle}{180}$$

Inputs	Letter	Explanation	Variable	Variable type
	angle	Angle of incidence	angle	double
Outputs	θ	Angle in terms of radian	Result	Double

```
Function teta(angle:Double):Double;
Begin
Result:=Pi*(angle/180);
End;
```

Table B.2: Angle of incidence for m^{th} mediums

$$\theta_m = \arcsin\left(\frac{N_0}{N_m} \sin\theta\right)$$

Inputs	Letter	Explanation	Variable	Variable type
	angle	Angle of incidence	angle	double
	N_0	Refractive index of air	N0	Double
	N_m	Refractive index of film	Nm	Double
Outputs	θ_m	Angle in terms of radian	Result	Double

```
Function steta(angle:Double; N0:Double; Nm:TC):TC;
Begin
Result:=CARCSIN(MulC(DivC(MakeC(N0,0),Nm),MakeC(sin(teta(angle)),0)));
End;
```

Table B.3: Calculation of delta function

$$\delta = \frac{2\pi N d \cos\theta}{\lambda}$$

	Letter	Explanation	Variable	Variable type
Inputs	N	Complex index $N = n - ik$	N	Complex
	d	Thickness of the film	d	Double
	θ	Angle of incidence	angle	Double
	λ	Wavelength in nm	lambda	Double
Outputs	δ	Delta value	Result	complex

```
Function delta(d:Double;N0:Double;Nm:TC;lambda:Double;angle:Double):TC;
Begin
Result:=MulC(MulC(MakeC(2*pi*d/lambda,0),Nm),CCos(steta(angle,N0,Nm)));
End;
```

Table B.4: Admittance of a film at P-polarization

$$\eta_m = \frac{\gamma N_m}{\cos\theta_m}$$

	Letter	Explanation	Variable	Variable type
Inputs	N_o	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	θ	Angle of incidence	angle	Double
Outputs	η	Admittance	Result	Complex

```
Function admittance_p(N0:Double; Nm:TC; angle:Double):TC;
Begin
Result:=DivC(mulC(MakeC(y,0),Nm),CCos(steta(angle,N0,Nm)));
End;
```

Table B.5: Admittance of medium at P-polarization

$$\eta_0 = \frac{\gamma N_0}{\cos\theta_0}$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of air	N0	Double
	θ	Incident angle	angle	Double
Outputs	η_0	Admittance of medium	Result	Complex

```
Function madmittance_p(N0:Double; angle:Double):Double;
Begin
Result:=y*N0/Cos(teta(angle));
End;
```

Table B.6: Admittance of substrate at P-polarization

$$\eta_s = \frac{\gamma N_s}{\cos\theta_s}$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of air	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	θ_0	Incident angle	angle	Double
Outputs	η_s	Admittance of substrate	Result	Complex

```
Function sadmittance_p(N0:Double; ns:TC; angle:Double):TC;
Begin
Result:=DivC(mulC(MakeC(y,0),ns),CCos(steta(angle,N0,ns)));
End;
```

Table B.7: m_{11} element of matrix at P-polarization

$$mp_{11} = \cos\delta_m$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	mp_{11}	mp11 element	Result	Complex

```
Function mp11(d:Double;N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=CCOS(delta(d,N0,Nm,lambda,angle));
End;
```

Table B.8: m_{12} element of matrix at P-polarization

$$mp_{12} = \frac{i\sin\delta_m}{\eta_m}$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	mp_{12}	mp21 element	Result	Complex

```
Function mp12(d:Double;N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=MulC(DivC(makeC(0,1),admittance_p(N0,Nm,angle)),CSin(delta(d,N0,Nm,lambda,angle)));
End;
```

Table B.9: m_{21} element of matrix at P-polarization

$$m_{21} = i\eta_m \sin \delta_m$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	mp_{21}	mp12 element	Result	Complex

```
Function mp21(d:Double;N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=MulC(MulC(makeC(0,1),admittance_p(N0,Nm,angle)),CSin(delta(d,N0,Nm,lambda,angle)));
End;
```

Table B.10: m_{22} element of matrix at P-polarization

$$mp_{22} = \cos \delta_m$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	mp_{22}	mp22 element	Result	Complex

```
Function mp22(d:Double;N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=CCOS(delta(d,N0,Nm,lambda,angle));
End;
```

Table B.11: B: Normalized electric field amplitude at P-polarization

$$B = m_{11} + m_{21}\eta_s$$

Inputs	Letter	Explanation	Variable	Variable type
	m_{11}	m11 element of matrix	m11	Complex
	m_{12}	m12 element of matrix	m21	Complex
	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	θ_0	Incident angle	angle	Double
Outputs	B_p	Normalized E-Field	Result	Complex

```
Function BpM(m11:TC;m12:TC;N0:Double;Ns:TC;angle:Double):TC ;
Begin
Result:=AddC(m11,MulC(m12,sadmittance_p(N0,Ns,angle)));
End;
```

Table B.12: C: Normalized magnetic field amplitude at P-polarization

$$C = m_{21} + m_{22}\eta_s$$

Inputs	Letter	Explanation	Variable	Variable type
	m_{21}	m12 element of matrix	m21	Complex
	m_{22}	m22 element of matrix	m22	Complex
	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	θ_0	Incident angle	angle	Double
Outputs	C_p	Normalized M-Field	Result	Complex

```
Function CpM(m21:TC;m22:TC;N0:Double;Ns:TC;angle:Double):TC ;
Begin
Result:=AddC(m21,MulC(m22,sadmittance_p(N0,Ns,angle)));
End;
```

Table B.13: Reflectance at P-polarization

$$R_q = \left(\frac{\eta_0 B - C}{\eta_0 B + C}\right)\left(\frac{\eta_0 B - C}{\eta_0 B + C}\right)^*$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	B	Normalized E-Field	B	Complex
	C	Normalized M-Field	C	Complex
	θ_0	Incident angle	angle	Double
Outputs	R_p	Reflectance	Result	Double

```
Function pRf(N0:Double;B:TC;C:TC;angle:Double):Double;
Var W:TC;
Begin
W:=DivC(SubC(MulC(makeC(madmittance_p(N0,angle),0),B),C),AddC(MulC(makeC(
    madmittance_p(N0,angle),0),B),C));
Result:=MulC(W,ConjugeC(W)).r;
End;
```

Table B.14: Transmittance at P-polarization

$$T_q = \frac{4\eta_0 Re(\eta_s)}{(\eta_0 B + C)(\eta_0 B + C)^*}$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	B	Normalized E-Field	B	Complex
	C	Normalized M-Field	C	Complex
	θ_0	Incident angle	angle	Double
Outputs	T_p	Transmittance	Result	Double

```
Function pTr(N0:Double;ns:TC;B:TC;C:TC;angle:Double):Double;
Var W,Q:TC;
Begin
W:=AddC(MulC(MakeC(madmittance_p(N0,angle),0),B),C);
Q:=MulC(makeC(madmittance_p(N0,angle),0),MakeC(4*sadmittance_p(n0,ns,angle).r,0));
Result:=DivC(Q,MulC(W,ConjugeC(W))).r;
End;
```

Table B.15: Absorptance at P-polarization

$$A_q = \frac{4\eta_0 Re(BC^* - \eta_s)}{(\eta_0 B+C)(\eta_0 B+C)^*}$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	B	Normalized E-Field	B	Complex
	C	Normalized M-Field	C	Complex
	θ_0	Incident angle	angle	Double
Outputs	A_p	Absorptance	Result	Double

```
Function pAb(N0:Double;ns:TC;B:TC;C:TC;angle:Double):Double;
Var W,Q:TC;
Begin
W:=AddC(MulC(makeC(madmittance_p(N0,angle),0),B),C);
Q:=MulC(makeC(madmittance_p(N0,angle),0),MakeC(4*subC(MulC(B,ConjugeC(C)),sadmittance_p(
    n0,ns,angle)).r,0));
Result:=DivC(Q,MulC(W,ConjugeC(W))).r;
End;
```

Table B.16: Admittance of a film at S-polarization

$$\eta_m = \gamma N_m \cos \theta_m$$

	Letter	Explanation	Variable	Variable type
Inputs	N_o	Refractive index of air	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	θ_0	Angle of incidence	angle	Double
Outputs	η_m	Admittance	Result	Complex

```
Function admittance_s(N0:Double; Nm:TC; angle:Double):TC;
Begin
Result:=MulC(mulC(MakeC(y,0),Nm),CCos(steta(angle,N0,Nm)));
End;
```

Table B.17: Admittance of medium at S-polarization

$$\eta_0 = \gamma N_0 \cos \theta_0$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	θ_0	Incident angle	angle	Double
Outputs	η_0	Admittance of medium	Result	Complex

```
Function madmittance_s(N0:Double; angle:Double):Double;
Begin
Result:=y*N0*Cos(teta(angle));
End;
```

Table B.18: Admittance of substrate at S-polarization

$$\eta_s = \gamma N_s \cos\theta_s$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	θ_0	Incident angle	angle	Double
Outputs	η_s	Admittance of substrate	Result	Complex

```
Function sadmittance_s(N0:Double; ns:TC; angle:Double):TC;
Begin
Result:=MulC(mulC(MakeC(y,0),ns),CCos(steta(angle,N0,ns)));
End;
```

Table B.19: m_{11} element of matrix at S-polarization

$$ms_{11} = \cos\delta_s$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	ms_{11}	ms11 element	Result	Complex

```
Function ms11(d:Double; N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=CCOS(delta(d,N0,Nm,lambda,angle));
End;
```

Table B.20: m_{12} element of matrix at S-polarization

$$ms_{12} = \frac{i \sin \delta_s}{\eta_s}$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	ms_{12}	ms12 element	Result	Complex

```
Function ms12(d:Double; N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=MulC(DivC(makeC(0,1),admittance_s(N0,Nm,angle)),CSin(delta(d,N0,Nm,lambda,angle)));
End;
```

Table B.21: m_{21} element of matrix at S-polarization

$$ms_{21} = i\eta_s \sin \delta_s$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	ms_{21}	ms12 element	Result	Complex

```
Function ms21(d:Double; N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=MulC(MulC(makeC(0,1),admittance_s(N0,Nm,angle)),CSin(delta(d,N0,Nm,lambda,angle)));
End;
```

Table B.22: m_{22} element of matrix at S-polarization

$$ms_{22} = \cos\delta_s$$

	Letter	Explanation	Variable	Variable type
Inputs	d	Thickness of the film	d	Double
	N_0	Refractive index of medium	N0	Double
	N_m	Refractive index of the film	Nm	Complex
	λ	Wavelength	lambda	Double
	θ_0	Incident angle	angle	Double
Outputs	ms_{22}	ms22 element	Result	Complex

```
Function ms22(d:Double; N0:Double; Nm:TC; lambda:Double;angle:Double):TC ;
Begin
Result:=CCOS(delta(d,N0,Nm,lambda,angle));
End;
```

Table B.23: B: Normalized electric field amplitude at S-polarization

$$B = m_{11} + m_{12}\eta_s$$

	Letter	Explanation	Variable	Variable type
Inputs	m_{11}	m11 element of matrix	m11	Complex
	m_{12}	m12 element of matrix	m21	Complex
	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	θ_0	Incident angle	angle	Double
Outputs	B_s	Normalized E-Field	Result	Complex

```
Function BsM(m11:TC;m12:TC;N0:Double;Ns:TC;angle:Double):TC ;
Begin
Result:=AddC(m11,MulC(m12,sadmittance_s(N0,Ns,angle)));
End;
```

Table B.24: C: Normalized magnetic field amplitude at S-polarization

$$C = m_{21} + m_{22}\eta_s$$

	Letter	Explanation	Variable	Variable type
Inputs	m_{21}	m21 element of matrix	m12	Complex
	m_{22}	m22 element of matrix	m22	Complex
	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	θ_0	Incident angle	angle	Double
Outputs	C_s	Normalized M-Field	Result	Complex

```
Function CsM(m21:TC;m22:TC;N0:Double;Ns:TC;angle:Double):TC ;
Begin
Result:=AddC(m21,MulC(m22,sadmittance_s(N0,Ns,angle)));
End;
```

Table B.25: Reflectance at S-polarization

$$R_s = \left(\frac{\eta_0 B-C}{\eta_0 B+C}\right)\left(\frac{\eta_0 B-C}{\eta_0 B+C}\right)^*$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	B	Normalized E-Field	B	Complex
	C	Normalized M-Field	C	Complex
	θ_0	Incident angle	angle	Double
Outputs	R_s	Reflectance	Result	Double

```
Function sRf(N0:Double;B:TC;C:TC;angle:Double):Double;
Var W:TC;
Begin
W:=DivC(SubC(MulC(makeC(madmittance_s(N0,angle),0),B),C),AddC(MulC(makeC(madmittance_s
    (N0,angle),0),B),C));
Result:=MulC(W,ConjugeC(W)).r;
End;
```

Table B.26: Transmittance at S-polarization

$$T_s = \frac{4\eta_0 Re(\eta_s)}{(\eta_0 B+C)(\eta_0 B+C)^*}$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	B	Normalized E-Field	B	Complex
	C	Normalized M-Field	C	Complex
	θ_0	Incident angle	angle	Double
Outputs	T_s	Transmittance	Result	Double

```
Function sTr(N0:Double;Ns:TC;B:TC;C:TC;angle:Double):Double;
Var W,Q:TC;
Begin
W:=AddC(MulC(MakeC(madmittance_s(N0,angle),0),B),C);
Q:=MulC(makeC(madmittance_s(N0,angle),0),MakeC(4*sadmittance_s(n0,ns,angle).r,0));
Result:=DivC(Q,MulC(W,ConjugeC(W))).r;
End;
```

Table B.27: Absorptance at S-polarization

$$A_s = \frac{4\eta_0 Re(BC^*-\eta_s)}{(\eta_0 B+C)(\eta_0 B+C)^*}$$

	Letter	Explanation	Variable	Variable type
Inputs	N_0	Refractive index of medium	N0	Double
	N_s	Refractive index of substrate	Ns	Complex
	B	Normalized E-Field	B	Complex
	C	Normalized M-Field	C	Complex
	θ_0	Incident angle	angle	Double
Outputs	A_s	Absorptance	Result	Double

```
Function sAb(N0:Double;ns:TC;B:TC;C:TC;angle:Double):Double;
Var W,Q:TC;
Begin
W:=AddC(MulC(makeC(madmittance_s(N0,angle),0),B),C);
Q:=MulC(makeC(madmittance_s(N0,angle),0),MakeC(4*subC(MulC(B,ConjugeC(C)),sadmittance_s(
    n0,ns,angle)).r,0));
Result:=DivC(Q,MulC(W,ConjugeC(W))).r;
End;
```

Appendix C

PROCEDURES OF MATRIX CALCULATION

Setting variables and arrays.

```
Procedure calculation(const lambda:wlarray; layers:layersarray; substrate:subsarray; thickness:tarray;
        angle:double);
var
msarray,mparray:array of array of TC;
xs1,xs2,xs3,xs4,ys1,ys2,ys3,ys4,Bs,Cs,xp1,xp2,xp3,xp4,yp1,yp2,yp3,yp4,Bp,Cp:TC;
sR,sT,sA,pR,pT,pA,mm:double;
i,j,N0:integer;
Begin
N0:=1;
SetLength(resultsarray,7,Length(layers));
SetLength(msarray,Length(layers[0]),4);
SetLength(mparray,Length(layers[0]),4);
```

Outer loop is used for scanning wavelength.

```
for i := 0 to Length(layers) − 1 do
Begin
```

Inner loop is used for a single wavelength for s-polarisation.

```
for j := 0 to Length(layers[0])−1 do
Begin
msarray[j,0]:=ms11(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
msarray[j,1]:=ms12(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
msarray[j,2]:=ms21(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
msarray[j,3]:=ms22(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
End;
```

Matrix multiplication.

```
xs1:=MakeC(1,0); xs2:=MakeC(0,0); xs3:=MakeC(0,0); xs4:=MakeC(1,0);
for j := 0 to Length(layers[1]) − 1 do
Begin
ys1:=AddC(MulC(xs1,msarray[j,0]),MulC(xs2,msarray[j,2]));
ys2:=AddC(MulC(xs1,msarray[j,1]),MulC(xs2,msarray[j,3]));
ys3:=AddC(MulC(xs3,msarray[j,0]),MulC(xs4,msarray[j,2]));
ys4:=AddC(MulC(xs3,msarray[j,1]),MulC(xs4,msarray[j,3]));
xs1:=ys1; xs2:=ys2; xs3:=ys3; xs4:=ys4;
End;
```

Resultant optical constants calculation.

```
Bs:=BsM(xs1,xs2,N0,MakeC(substrate[i,0],−substrate[i,1]),angle);
Cs:=CsM(xs3,xs4,N0,MakeC(substrate[i,0],−substrate[i,1]),angle);
resultsarray[0,i]:=lambda[i];
sR:=sRf(n0,Bs,Cs,angle);
resultsarray[1,i]:=sR;
sT:=sTr(N0,MakeC(substrate[i,0],−substrate[i,1]),Bs,Cs,angle);
resultsarray[3,i]:=sT;
sA:=sAb(N0,MakeC(substrate[i,0],−substrate[i,1]),Bs,Cs,angle);
resultsarray[5,i]:=sA;
End;
```

Inner loop is used for a single wavelength for p-polarisation.

```
for i := 0 to Length(layers) − 1 do
Begin
for j := 0 to Length(layers[0])−1 do
Begin
mparray[j,0]:=mp11(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
mparray[j,1]:=mp12(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
mparray[j,2]:=mp21(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
mparray[j,3]:=mp22(thickness[j],N0,MakeC(layers[i,j,0],−layers[i,j,1]),lambda[i],angle);
End;
```

Matrix multiplication.

```
xp1:=MakeC(1,0); xp2:=MakeC(0,0); xp3:=MakeC(0,0); xp4:=MakeC(1,0);
for j := 0 to Length(layers[1]) − 1 do
Begin
yp1:=AddC(MulC(xp1,mparray[j,0]),MulC(xp2,mparray[j,2]));
yp2:=AddC(MulC(xp1,mparray[j,1]),MulC(xp2,mparray[j,3]));
yp3:=AddC(MulC(xp3,mparray[j,0]),MulC(xp4,mparray[j,2]));
yp4:=AddC(MulC(xp3,mparray[j,1]),MulC(xp4,mparray[j,3]));
xp1:=yp1; xp2:=yp2; xp3:=yp3; xp4:=yp4;
End;
```

Resultant optical constants calculation.

```
Bp:=BpM(xp1,xp2,N0,MakeC(substrate[i,0],−substrate[i,1]),angle);
Cp:=CpM(xp3,xp4,N0,MakeC(substrate[i,0],−substrate[i,1]),angle);
resultsarray[0,i]:=lambda[i];
pR:=pRf(n0,Bp,Cp,angle);
resultsarray[2,i]:=pR;
pT:=pTr(N0,MakeC(substrate[i,0],−substrate[i,1]),Bp,Cp,angle);
resultsarray[4,i]:=pT;
pA:=pAb(N0,MakeC(substrate[i,0],−substrate[i,1]),Bp,Cp,angle);
resultsarray[6,i]:=pA;
End;
```

End of inner loop

```
End;
```

Appendix D

PROCEDURES FOR PLOTTING

Plotting the results on a picture area.

```
Procedure grafik(CONST image:Timage; gl,gsr,gpr,gst,gpt,gsa,gpa:array of double);
```

Adjusting graphic constants.

```
Const
xSize = 570;
ySize = 270;
gx=45;
gy=230;
gw=505;
gh=205;
Var
Bitmap : TBitmap;
i:integer;
Begin
Bitmap := TBitmap.Create;
```

Sketching of graph and inserting labels.

```
Try
Bitmap.Width := xSize;
Bitmap.Height := ySize;
Bitmap.PixelFormat := pf24bit;
Bitmap.Canvas.Pen.Color:=clBlack;
Bitmap.Canvas.MoveTo(gx−5,gy);
Bitmap.Canvas.LineTo(gx+gw,gy);
Bitmap.Canvas.MoveTo(gx−5,gy−gh+5);
Bitmap.Canvas.LineTo(gx+gw,gy−gh+5);
Bitmap.Canvas.MoveTo(gx,gy);
Bitmap.Canvas.LineTo(gx,gy−gh);
```

```
Bitmap.Canvas.MoveTo(gx+gw−5,gy);
Bitmap.Canvas.LineTo(gx+gw−5,gy−gh);
Bitmap.Canvas.Font.Name:='Times New Roman';
Bitmap.Canvas.Font.Size:=8;
Bitmap.Canvas.TextOut(gx+gw−80,gy+20,'WaveLength [nm]');

for i := 0 to 10 do
Begin
Bitmap.Canvas.MoveTo(gx+50*i,gy);
Bitmap.Canvas.LineTo(gx+50*i,gy+5);
Bitmap.Canvas.MoveTo(gx+25+50*i,gy);
Bitmap.Canvas.LineTo(gx+25+50*i,gy+3);
Bitmap.Canvas.MoveTo(gx+50*i,gy−gh+5);
Bitmap.Canvas.LineTo(gx+50*i,gy−gh);
Bitmap.Canvas.MoveTo(gx+25+50*i,gy−gh+5);
Bitmap.Canvas.LineTo(gx+25+50*i,gy−gh+2);
Bitmap.Canvas.MoveTo(gx+gw−5,gy−20*i);
Bitmap.Canvas.LineTo(gx+gw−2,gy−20*i);
Bitmap.Canvas.TextOut(gx−10+50*i,gy+5,IntToStr(200+100*i));
Bitmap.Canvas.MoveTo(gx,gy−20*i);
Bitmap.Canvas.LineTo(gx−5,gy−20*i);
Bitmap.Canvas.TextOut(gx−22,gy−7−20*i,IntToStr(10*i));
End;

Bitmap.Canvas.Font.Style:=[fsBold];
Bitmap.Canvas.Font.Color:=clRed;
Bitmap.Canvas.TextOut(gx−25,gy−gh−20,'R');
Bitmap.Canvas.Font.Color:=clLime;
Bitmap.Canvas.TextOut(gx−5,gy−gh−20,'T');
Bitmap.Canvas.Font.Color:=clblue;
Bitmap.Canvas.TextOut(gx+15,gy−gh−20,'A');
Bitmap.Canvas.Font.Color:=clBlack;
Bitmap.Canvas.Font.Style:=[];
Bitmap.Canvas.Pen.Color:=clRed;
```

Plotting the results.

```
for i := 0 to length(gl)−2 do
Begin
Bitmap.Canvas.MoveTo(gx+round((gl[i]−200)/2),gy−2∗round(100∗gsr[i]));
Bitmap.Canvas.LineTo(gx+round((gl[i+1]−200)/2),gy−2∗round(100∗gsr[i+1]));
Bitmap.Canvas.MoveTo(gx+round((gl[i]−200)/2),gy−2∗round(100∗gpr[i]));
Bitmap.Canvas.LineTo(gx+round((gl[i+1]−200)/2),gy−2∗round(100∗gpr[i+1]));
End;
Bitmap.Canvas.Pen.Color:=clLime;
for i := 0 to length(gl)−2 do
Begin
Bitmap.Canvas.MoveTo(gx+round((gl[i]−200)/2),gy−2∗round(100∗gst[i]));
Bitmap.Canvas.LineTo(gx+round((gl[i+1]−200)/2),gy−2∗round(100∗gst[i+1]));
Bitmap.Canvas.MoveTo(gx+round((gl[i]−200)/2),gy−2∗round(100∗gpt[i]));
Bitmap.Canvas.LineTo(gx+round((gl[i+1]−200)/2),gy−2∗round(100∗gpt[i+1]));
End;
Bitmap.Canvas.Pen.Color:=clBlue;
for i := 0 to length(gl)−2 do
Begin
Bitmap.Canvas.MoveTo(gx+round((gl[i]−200)/2),gy−2∗round(100∗gsa[i]));
Bitmap.Canvas.LineTo(gx+round((gl[i+1]−200)/2),gy−2∗round(100∗gsa[i+1]));
Bitmap.Canvas.MoveTo(gx+round((gl[i]−200)/2),gy−2∗round(100∗gpa[i]));
Bitmap.Canvas.LineTo(gx+round((gl[i+1]−200)/2),gy−2∗round(100∗gpa[i+1]));
End;
Bitmap.Canvas.Font.Size:=8;
if (gsr[100]−gpr[100])>0.1 then
Begin
Bitmap.Canvas.TextOut(550,gy−2∗round(100∗gpr[100]),'TE');
Bitmap.Canvas.TextOut(550,gy−2∗round(100∗gsr[100]),'TM');
Bitmap.Canvas.TextOut(550,gy−2∗round(100∗gpt[100]),'TE');
Bitmap.Canvas.TextOut(550,gy−2∗round(100∗gst[100]),'TM');
Bitmap.Canvas.TextOut(550,gy−2∗round(100∗gpa[100]),'TE');
Bitmap.Canvas.TextOut(550,gy−2∗round(100∗gsa[100]),'TM');
End;
Image.Picture.Graphic := Bitmap;
Finally
Bitmap.Free
End;
End;
```