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A polynomial approach for reflection, transmission, and ellipsometric parameters by isotropic stratified media

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A polynomial approach for the calculation of the reflectance, the transmittance, and the ellipsometric parameters of a stratified isotropic planar structure is presented. We show that these parameters can be written in a very simple and compact form using the so-called elementary symmetric functions that are extensively used in the mathematical theory of polynomials. This approach is applied to quarter-wave Bragg reflectors. The numerical results reveal an exact match with the well known matrix formalism.

Keywords: ellipsometry, reflectance, transmittance, ellipsometric parameters, quarter-wave Bragg reflectors, stratified planar structure.

1. Introduction

Ellipsometry offers a precise technique for measuring thin film properties. Advanced ellipsometers have shown an excellent sensitivity for monitoring the growth of optical films during film deposition. DRUDE [1] was the first to build an ellipsometer even before the word "ellipsometry" was coined in 1954. In the aftermath, the equipment built by Drude received little attention for decades until the 1970's, ellipsometry received an increasing interest and a considerable number of papers on ellipsometry have been published [2–5].

Ellipsometry measures the changes in the state of polarization of light upon reflection or transmission from a sample. It has a number of advantages over traditional intensity reflection and transmission measurements. Some of these advantages lie in that it measures an intensity ratio and therefore it is less affected by intensity instabilities of the light source. It also measures at least two parameters at each wavelength.

The ellipsometric results are usually presented in terms of two parameters ψ and Δ given by

$$\rho = \tan(\psi)\exp(i\Delta) = \frac{r_p}{r_s} \tag{1}$$

where r_p and r_s are the complex Fresnel reflection coefficients for *p*- and *s*-polarized light, respectively.

This paper addresses the use of a polynomial approach for the study of reflectance, transmittance, and ellipsometric parameters ψ and Δ for any number of isotropic multilayer structures. Some examples of these structures are ITO on glass, SiO_2 on silicon, and HfO_2 on silicon. We first present the conventional matrix method, then we introduce the so-called elementary symmetric functions used in the mathematical theory of polynomials to write the reflection and transmission coefficients in a simple and compact form.

2. Matrix representation for the reflection and transmission coefficients

Consider the case where a beam of light is incident on a multilayer structure of $(N+1)$ isotropic media, as shown in Fig. 1. The j-th medium has d_j and n_j as a thickness and a refractive index, respectively. The j-th interface located at z_j separates the two media of refractive indices n_j and n_{j+1}.

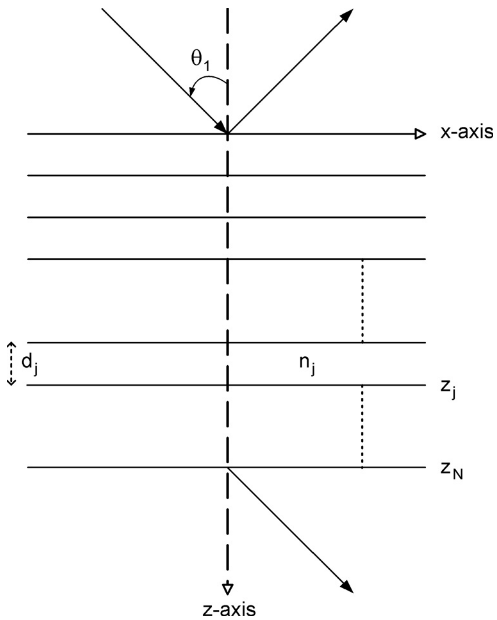


Fig. 1. A structure of $(N+1)$ stratified planar media.

In general, the total field can be written as

$$E(z) = \begin{pmatrix} E^+(z) \\ E^-(z) \end{pmatrix} \tag{2}$$

where $E^+(z)$ and $E^-(z)$ denote the complex amplitudes of the forward and the backward--traveling plane waves at an arbitrary plane z. If we consider the fields at two different planes parallel to the interfaces, then the fields E_1 and E_N are related by a transformation matrix $[M]$ according to the following equation [6]

$$\begin{pmatrix} E_1^+ \\ E_1^- \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} E_N^+ \\ E_N^- \end{pmatrix} \tag{3}$$

For the last interface we have $E_N^- = 0$. So, the reflection and transmission coefficients of the whole system are given by

$$\left.\begin{aligned} r_N &= \frac{E_1^-}{E_1^+} = \frac{M_{21}}{M_{11}} \\ t_N &= \frac{E_N^+}{E_1^+} = \frac{1}{M_{11}} \end{aligned}\right\} \tag{4}$$

The Fresnel reflection and transmission coefficients $r_{j,j+1}$ and $t_{j,j+1}$ at the $j, j+1$ interface for s- and p-polarizations are given by [6]

$$r_{j,j+1}^s = \frac{n_j \cos\theta_j - n_{j+1}\cos\theta_{j+1}}{n_j \cos\theta_j + n_{j+1}\cos\theta_{j+1}} \tag{5}$$

$$t_{j,j+1}^s = \frac{2n_j \cos\theta_j}{n_j \cos\theta_j + n_{j+1}\cos\theta_{j+1}} \tag{6}$$

$$r_{j,j+1}^p = \frac{n_{j+1} \cos\theta_j - n_j\cos\theta_{j+1}}{n_{j+1} \cos\theta_j + n_j\cos\theta_{j+1}} \tag{7}$$

$$t_{j,j+1}^p = \frac{2n_j \cos\theta_j}{n_{j+1} \cos\theta_j + n_j\cos\theta_{j+1}} \tag{8}$$

The matrix $[M]$ can be expressed as the product of interface matrices and layer matrices. The matrix $[r_j^\alpha]$ of the j-th interface located at the plane z_j between two layers of refractive indices n_j and n_{j+1} relates the fields on both sides of the interface, *i.e.*,

$$E^{\alpha}(z_j - \varepsilon) = \left[r_j^{\alpha}\right] E^{\alpha}(z_j + \varepsilon) \tag{9}$$

where α stands for p in p-polarization and for s in s-polarization, and ε is an infinitely small distance. The interface matrix is given by

$$\left[r_j^{\alpha}\right] = \frac{1}{t_{j,j+1}^{\alpha}} \begin{bmatrix} 1 & r_{j,j+1}^{\alpha} \\ r_{j,j+1}^{\alpha} & 1 \end{bmatrix} \tag{10}$$

The propagation of the fields across the same layer with refractive index n_j between two interfaces located at z_{j-1} and $z_j = z_{j-1} + d_j$ is given by the matrix $[\phi_j]$, *i.e.*,

$$E^{\alpha}(z_{j-1} + \varepsilon) = [\phi_j]\, E^{\alpha}(z_j - \varepsilon) \tag{11}$$

where the matrix $[\phi_j]$ is given by

$$\left[\phi_j\right] = \begin{pmatrix} e^{i\varphi_j} & 0 \\ 0 & e^{-i\varphi_j} \end{pmatrix} \tag{12}$$

and $\varphi_j = k_o n_j d_j \cos(\theta_j)$, with k_o being the free space wave number.

The M-matrix of such a system can be written as the product

$$\left[M_N^{\alpha}\right] = \left[\phi_1\right]\left[r_1^{\alpha}\right]\left[\phi_2\right]\left[r_2^{\alpha}\right]\ldots\left[\phi_N\right]\left[r_N^{\alpha}\right] \tag{13}$$

3. Polynomial approach

The interface and layer matrices have the following commutation relation [7, 8]

$$\left[\phi_j\right]\left[r_j^{\alpha}\right] = \left[r_j^{\alpha}(\varphi_j)\right]\left[\phi_j\right] \tag{14}$$

The matrix $[r_j^{\alpha}(\varphi_j)]$ is obtained by adding a phase term $\exp(\pm 2i\varphi_j)$ to the element $r_{j,j+1}^{\alpha}$ in the matrix $[r_j^{\alpha}]$ in Eq. (10), *i.e.*,

$$\left[r_j^{\alpha}(\varphi_j)\right] = \frac{1}{t_{j,j+1}^{\alpha}} \begin{bmatrix} 1 & r_{j,j+1}^{\alpha} e^{2i\varphi_j} \\ r_{j,j+1}^{\alpha} e^{-2i\varphi_j} & 1 \end{bmatrix} \tag{15}$$

It is more convenient to introduce the matrix

$$\left[r_j^\alpha(\varphi_1 + \varphi_2 + \dots + \varphi_j)\right] = \frac{1}{t_{j,j+1}^\alpha}\begin{bmatrix} 1 & r_{j,j+1}^\alpha e^{2i(\varphi_1 + \varphi_2 + \dots + \varphi_j)} \\ r_{j,j+1}^\alpha e^{-2i(\varphi_1 + \varphi_2 + \dots + \varphi_j)} & 1 \end{bmatrix} \tag{16}$$

and to define

$$\left.\begin{aligned} R_j^\alpha \equiv R_{j,j+1}^\alpha &= r_{j,j+1}^\alpha e^{-2i(\varphi_1 + \varphi_2 + \dots + \varphi_j)} \\ \bar{R}_j^\alpha \equiv \bar{R}_{j,j+1}^\alpha &= r_{j,j+1}^\alpha e^{2i(\varphi_1 + \varphi_2 + \dots + \varphi_j)} \end{aligned}\right\} \tag{17}$$

where the overbar on R denotes the change of φ_j into $-\varphi_j$. According to Eq. (16) and Eq. (17) we can write a new matrix

$$\left[R_j^\alpha\right] = \frac{1}{t_{j,j+1}^\alpha}\begin{bmatrix} 1 & \bar{R}_{j,j+1}^\alpha \\ R_{j,j+1}^\alpha & 1 \end{bmatrix} \tag{18}$$

The interesting feature of Eqs. (16) and (17) is the phase term $\exp(\pm 2i\varphi_j)$ multiplied by the element $r_{j,j+1}^\alpha$ which means that each interface takes into account the entire history of the wave due to all layers up to the j-th interface.

In view of the commutation relation given by Eqs. (14), (17) and (18) we can write any product of $[r_j^\alpha]$ and $[\phi_j]$ matrices in such a form that all the layer matrices $[\phi_j]$ are located to the right of all the interface matrices $[r_j^\alpha]$. Thus, Eq. (13) can be rewritten as [7–9]

$$\left[M_N^\alpha\right] = \left[R_1^\alpha\right]\left[R_2^\alpha\right]\left[R_3^\alpha\right]\dots\left[R_N^\alpha\right]\left[\phi_1 + \phi_2 + \dots + \phi_N\right] \tag{19}$$

where

$$\left[\phi_1\right]\left[\phi_2\right]\dots\left[\phi_N\right] = \left[\phi_1 + \phi_2 + \dots + \phi_N\right] \tag{20}$$

Let the product of the $[R_j^\alpha]$ matrices in Eq. (19) be given by a matrix $[D_N^\alpha]$, *i.e.*,

$$\left[D_N^\alpha\right] = \left[R_1^\alpha\right]\left[R_2^\alpha\right]\dots\left[R_N^\alpha\right] \tag{21}$$

It has been shown [7–9] that the elements of the matrix $[D_N^\alpha]$ can be written using a complex generalization of the symmetric functions of the mathematical theory of polynomials [10, 11] as follows

$$\left[D_N^{\alpha}\right] = \frac{1}{\prod_{j=1}^{N} t_{j,j+1}^{\alpha}} \begin{bmatrix} \sum_{m \geq 0} \left(\overline{S_{2m}^{\alpha,N}}\right) & \sum_{m \geq 0} \left(\overline{S_{2m+1}^{\alpha,N}}\right) \\ \sum_{m \geq 0} \left(S_{2m+1}^{\alpha,N}\right) & \sum_{m \geq 0} \left(S_{2m}^{\alpha,N}\right) \end{bmatrix} \tag{22}$$

where

$$S_0^{\alpha,N} = 1 \tag{23a}$$

$$S_1^{\alpha,N} = \sum_{i=1}^{N} R_i^{\alpha} = R_1^{\alpha} + R_2^{\alpha} + \ldots + R_N^{\alpha} \tag{23b}$$

$$S_2^{\alpha,N} = \sum_{1 \leq i < j \leq N} R_i^{\alpha} \overline{R}_j^{\alpha} = R_1^{\alpha} \overline{R}_2^{\alpha} + R_1^{\alpha} \overline{R}_3^{\alpha} + \ldots + R_1^{\alpha} \overline{R}_N^{\alpha} + + R_2^{\alpha} \overline{R}_3^{\alpha} + R_2^{\alpha} \overline{R}_4^{\alpha} + \ldots + R_2^{\alpha} \overline{R}_N^{\alpha} + \ldots + R_{N-1}^{\alpha} \overline{R}_N^{\alpha} \tag{23c}$$

$$S_3^{\alpha,N} = \sum_{1 \leq i < j < k \leq N} R_i^{\alpha} \overline{R}_j^{\alpha} R_k^{\alpha} = R_1^{\alpha} \overline{R}_2^{\alpha} R_3^{\alpha} + R_1^{\alpha} \overline{R}_2^{\alpha} R_4^{\alpha} + \ldots + + R_1^{\alpha} \overline{R}_2^{\alpha} R_N^{\alpha} + \ldots + R_{N-2}^{\alpha} \overline{R}_{N-1}^{\alpha} R_N^{\alpha} \tag{23d}$$

$$S_P^{\alpha,N} = \sum_{1 \leq i < j < k < \ldots < w \leq N} R_i^{\alpha} \overline{R}_j^{\alpha} R_k^{\alpha} \overline{R}_1^{\alpha} \ldots \overset{0}{R}{}_w^{\alpha} \tag{23e}$$

where P – terms in each sum. Equations (23) defines the elementary symmetric functions of the variables $R_1^{\alpha}, R_2^{\alpha}, R_3^{\alpha}, \ldots, R_N^{\alpha}$.

At this point, we emphasize the following:

1. As mentioned above, the overbar in $\overline{R}$ denotes the change of φ_j into $-\varphi_j$;
2. S_P is the sum of all possible products of P-terms R_j;
3. In each product term of Eqs. (23), the factors R and $\overline{R}$ appear alternatively with the first factor being always R. This remark gives the meaning of $\overset{0}{R}$, that is, R when the place of $\overset{0}{R}$ in the product is odd and $\overline{R}$ when the place of $\overset{0}{R}$ is even;
4. $S_P^{\alpha,N} = 0$ for $P > N$.

Now, we can write the M-matrix, given by Eq. (19), as

$$\left[M_N^{\alpha}\right] = \frac{1}{\prod_{j=1}^{N} t_{j,j+1}^{\alpha}} \begin{bmatrix} \sum_{m \geq 0} \left(\overline{S_{2m}^{\alpha,N}}\right) e^{i(\varphi_1 + \varphi_2 + \ldots + \varphi_N)} & \sum_{m \geq 0} \left(\overline{S_{2m+1}^{\alpha,N}}\right) e^{-i(\varphi_1 + \varphi_2 + \ldots + \varphi_N)} \\ \sum_{m \geq 0} \left(S_{2m+1}^{\alpha,N}\right) e^{i(\varphi_1 + \varphi_2 + \ldots + \varphi_N)} & \sum_{m \geq 0} \left(S_{2m}^{\alpha,N}\right) e^{-i(\varphi_1 + \varphi_2 + \ldots + \varphi_N)} \end{bmatrix} \tag{24}$$

Equation (24) enables us to write the overall reflection and transmission coefficients of the isotropic planar stratified structure in the general form

$$r_N^\alpha = \frac{M_{21}^\alpha}{M_{11}^\alpha} = \frac{\sum\limits_{m \geq 0} S_{2m+1}^{\alpha, N}}{\sum\limits_{m \geq 0} \left(\overline{S_{2m}^{\alpha, N}} \right)} \tag{25}$$

$$t_N^\alpha = \frac{1}{M_{11}^\alpha} = \frac{\prod\limits_{j=1}^{N} t_{j, j+1}^\alpha}{\sum\limits_{m \geq 0} \left(\overline{S_{2m}^{\alpha, N}} \right) e^{i(\varphi_1 + \varphi_2 + \ldots + \varphi_N)}} \tag{26}$$

Moreover, the ellipsometric parameters ψ and Δ are then given by

$$\tan(\psi) e^{i\Delta} = \frac{r_N^p}{r_N^s} = \frac{\sum\limits_{m \geq 0} S_{2m+1}^{p, N} \sum\limits_{m \geq 0} \left(\overline{S_{2m}^{s, N}} \right)}{\sum\limits_{m \geq 0} S_{2m+1}^{s, N} \sum\limits_{m \geq 0} \left(\overline{S_{2m}^{p, N}} \right)} \tag{27}$$

4. Numerical applications and results

To demonstrate the validity of the polynomial approach we consider a planar multilayer dielectric coating designed as a dielectric mirror. Dielectric mirrors (also known as Bragg reflectors) have received an increasing interest due to their extremely low losses at optical and infrared frequencies, as compared to ordinary metallic mirrors. A dielectric mirror usually consists of identical alternating layers of high and low refractive indices, as shown in Fig. 2. The optical thicknesses are typically chosen

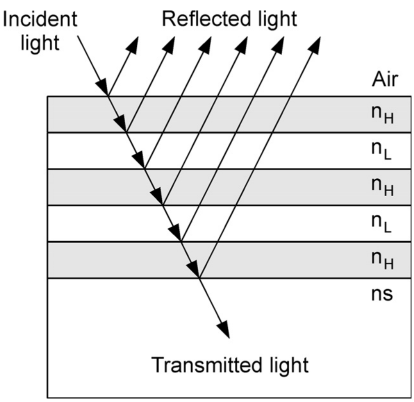


Fig. 2. Five-layer quarter-wave Bragg reflector (dielectric mirror).

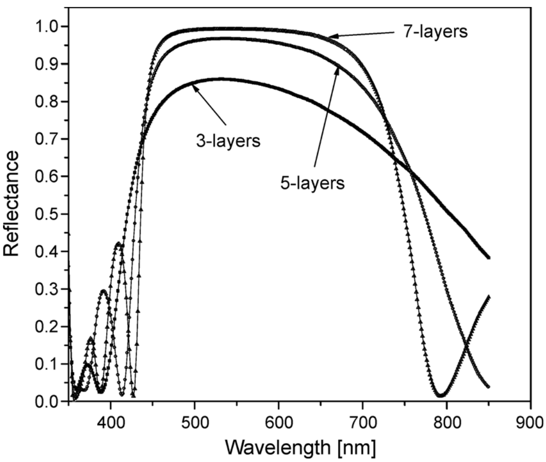


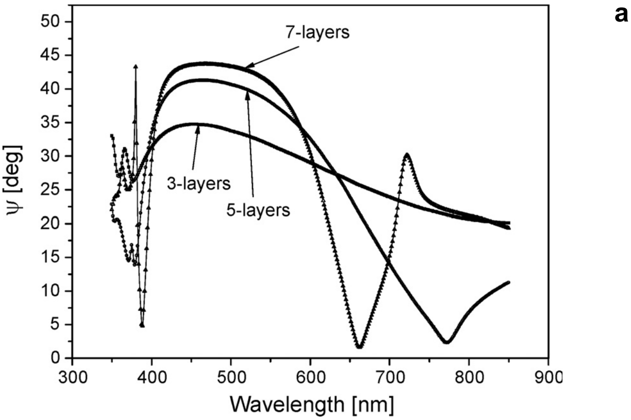
Fig. 3. Calculated reflectance of 3, 5, 7 quarter-wavelength layer Bragg reflectors at normal incidence in the spectral range of 350−850 nm for the polynomial approach (points) and the matrix formulation (solid lines).

to be quarter-wavelength long at some center wavelength λ_o, that is, $n_H d_H = n_L d_L = \lambda_o/4$, where n_H and n_L are the indices of refraction of the high- and low-index layers, respectively, d_H and d_L are the thicknesses of the high- and low-index layers, respectively. The standard arrangement is to have an odd number of layers, with the high index layer being the first and last layer [12].

The numerical calculation is done for a system of $(2K + 1)$ stack of quarter-wavelength layers where $K = 1, 2$, and 3. The design wavelength of the Bragg reflectors (filter) is centered at 550 nm. The reflectance and the ellipsometric parameters ψ and Δ were calculated using the well known matrix formulation [6] and the model proposed. These calculations were performed for the systems under consideration in the spectral range from 350 to 850 nm. The indices n_H and n_L correspond to layers of TiO_2 and MgF_2 on a glass substrate. The optical parameters of these layers were obtained from the handbook of optical constants of solids [13, 14]. The results are depicted in Figs. 3 and 4. The calculated overall reflectance of 3, 5, and 7 layer Bragg reflectors centered at $\lambda_o = 550$ nm are plotted in Fig. 3. The figure reveals an exact match between the polynomial and matrix formalisms. The ellipsometric parameters ψ and Δ are depicted in Fig. 4 for the same reflectors mentioned above. A complete agreement between the two approaches is obvious.

5. Conclusions

In this article, we have shown that the reflectance, transmittance, and the ellipsometric parameters can be calculated for any stack of layers using a simple method utilizing the elementary symmetric functions. This approach exhibits an excellent agreement



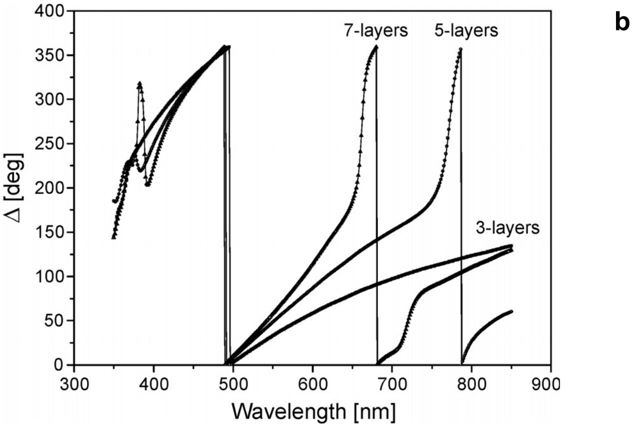


Fig. 4. Calculated ψ (**a**) and Δ (**b**) of 3, 5, 7 quarter-wavelength layer Bragg reflectors at a 70° angle of incidence in the spectral range of 350–850 nm for the polynomial approach (points) and the matrix formulation (solid lines).

with the traditional matrix method for a system representing a dielectric mirror. We believe that this method is much easier than the traditional matrix multiplication method.

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