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In this review paper a uniform matrix formalism enabling us to include the important defects of thin film systems into the formulae for their optical quantities is presented. The following defects are discussed: roughness of the boundaries; inhomogeneity represented by profiles of the refractive indices; transition interface layers and volume inhomogeneity. It is shown that this formalism is relatively very efficient. This fact is demonstrated using a theoretical example representing a complicated thin film system exhibiting defects.

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**1 Introduction**

In practice thin film systems with various defects are often encountered. There are several defects influencing enormously the optical properties of these systems. In this contribution the influence of the most important defects on the optical quantities characterizing the thin film systems will be presented. Thus the attention will be devoted to the influence of roughness of the boundaries, inhomogeneity represented by profiles of the refractive indices, transition interface layers and volume inhomogeneity on the values of the optical quantities of the thin film systems will be discussed.

It will be shown that the uniform  $2 \times 2$  matrix formalism can be used to derive the formulae expressing the main optical quantities of the systems mentioned exhibiting the defects introduced. This means that within this matrix formalism the formulae for the ellipsometric parameters, reflectances and transmittances of the thin films with the defect mentioned will be presented.

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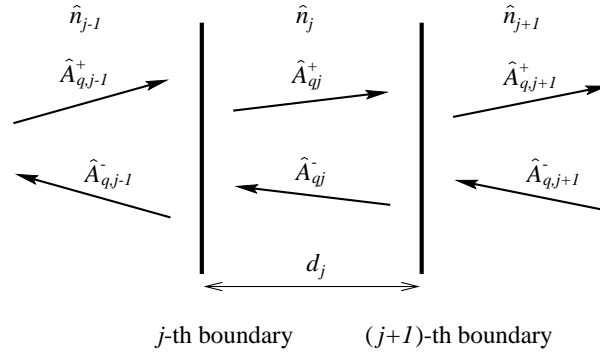


Fig. 1. Schematic diagram of the  $j$ -th film of the isotropic thin film system.

## 2 Ideal isotropic thin film systems

In the isotropic thin film systems the materials forming the individual media are characterized by the complex refractive indices. Every monochromatic plane wave propagating within the optically isotropic medium can be expressed by a superposition of two linearly polarized waves. If these two linearly polarized waves are chosen so that the first of them is polarized perpendicularly to the plane of incidence (s-polarization) and the latter one is parallel with this plane (p-polarization) it is possible to separate the solution of the Maxwell equations corresponding to the system considered to two particular solutions belonging to these p- and s-polarized waves.

The boundary conditions for the electromagnetic fields give the following matrix equation for the  $j$ -th boundary of the system:

$$\vec{A}_{q,j-1} = \tilde{B}_{qj} \vec{A}_{qj}, \quad q = \text{p or s}, \quad (1)$$

where  $\vec{A}_{qj}$  denotes the vector whose components are formed by the complex amplitudes  $\hat{A}_{qj}^+$  and  $\hat{A}_{qj}^-$  of the electric fields belonging to the right-going and left-going waves inside of the  $j$ -th film, respectively (see Fig. 1), i. e.

$$\vec{A}_{qj} = \begin{pmatrix} \hat{A}_{qj}^+ \\ \hat{A}_{qj}^- \end{pmatrix}. \quad (2)$$

The *refraction matrix*  $\tilde{B}_{qj}$  is defined as follows:

$$\tilde{B}_{qj} = \frac{1}{\hat{t}_{qj}} \begin{pmatrix} 1 & \hat{r}_{qj} \\ \hat{r}_{qj} & 1 \end{pmatrix}. \quad (3)$$

This matrix expresses the binding conditions for the amplitudes mentioned at the  $j$ -th boundary. The symbols  $\hat{r}_{qj}$  and  $\hat{t}_{qj}$  represent the Fresnel reflection and transmission coefficients, respectively, for the wave incident on the boundary from the left side [1, 2].

The amplitudes of the waves inside of the  $j$ -th film corresponding to the  $j$ -th and  $(j+1)$ -th boundaries are connected with the elements of the *phase matrix*  $\tilde{T}_j$ , i. e.

$$\tilde{T}_j = \begin{pmatrix} e^{i\hat{X}_j} & 0 \\ 0 & e^{-i\hat{X}_j} \end{pmatrix}, \quad (4)$$

where

$$\hat{X}_j = \frac{2\pi}{\lambda} d_j \sqrt{\hat{n}_j^2 - \sin^2 \theta_0}. \quad (5)$$

In the foregoing equation the symbols  $d_j$  and  $\hat{n}_j$  represent the thickness and the complex refractive index of the  $j$ -th film, respectively. The symbols  $\lambda$  and  $\theta_0$  denote the wavelength of incident light and angle of incidence, respectively.

For the ideal isotropic thin film systems containing  $N$  films one can write the following matrix equation:

$$\vec{A}_{q0} = \tilde{B}_{q1} \tilde{T}_1 \tilde{B}_{q2} \tilde{T}_2 \dots \tilde{B}_{qN} \tilde{T}_N \tilde{B}_{q,N+1} \vec{A}_q = \tilde{M}_q \vec{A}_q, \quad (6)$$

where the vectors  $\vec{A}_{q0}$  and  $\vec{A}_q$  exhibit the special form if the wave with the amplitude equal to unity falls on the system considered, i. e.

$$\vec{A}_{q0} = \begin{pmatrix} 1 \\ \hat{r}_q \end{pmatrix}, \quad \vec{A}_q = \begin{pmatrix} \hat{t}_q \\ 0 \end{pmatrix}. \quad (7)$$

The symbols  $\hat{r}_q$  and  $\hat{t}_q$  denote the Fresnel coefficients for reflected and transmitted waves by the system, respectively. From the foregoing it is apparent that they are determined as follows (see Eq. (6)):

$$\hat{r}_q = \frac{\hat{M}_{q21}}{\hat{M}_{q11}} \quad \text{and} \quad \hat{t}_q = \frac{1}{\hat{M}_{q11}}. \quad (8)$$

The matrix  $\tilde{M}_q$  is called the *overall transfer matrix* of the thin film system.

The ellipsometric parameters  $\Psi$  (azimuth) and  $\Delta$  (phase change) characterizing the ideal isotropic thin film system can then be calculated using the following equations:

$$\tan \Psi e^{i\Delta} = \frac{\hat{r}_p}{\hat{r}_s} \quad \text{or} \quad \tan \Psi e^{i\Delta} = \frac{\hat{t}_p}{\hat{t}_s}. \quad (9)$$

The reflectances  $R_q$  and transmittances  $T_q$  for both the polarizations are given as follows:

$$R_q = |\hat{r}_q|^2 \quad \text{and} \quad T_q = \frac{n \cos \theta}{\cos \theta_0} |\hat{t}_q|^2, \quad (10)$$

where the symbols  $n$  and  $\theta_0$  represent the refractive index and refraction angle corresponding to the substrate. For ideally unpolarized light (natural light) the reflectance  $R$  and transmittance  $T$  are expressed in the following way:

$$R = \frac{1}{2}(R_p + R_s) \quad \text{and} \quad T = \frac{1}{2}(T_p + T_s). \quad (11)$$

### 3 Systems exhibiting defects

In this section the influence of the important defects on the optical properties of the thin film systems will be described briefly.

### 3.1 Microrough boundaries

If the boundaries of the thin film systems can be represented by the model of microrough surface (MCRS) one can employ some of the formulae of the theory of effective medium for expressing the optical quantities of these systems. For the model of MCRS the following relations are fulfilled:  $\sigma \ll \lambda$  and  $T \ll \lambda$  ( $\sigma$  and  $T$  denote the RMS value of the heights of the irregularities and autocorrelation length of these irregularities [3]). Within the theory mentioned one can replace the microrough boundaries by fictitious films with suitable “effective” optical constants and thicknesses. The boundaries of these fictitious thin films are ideally smooth. The effective optical constants of the fictitious films depend on the structure of the corresponding rough boundaries. In the first approximation these fictitious films can be represented by isotropic and homogeneous layers. Then the optical constants of the fictitious films are expressed using some formula of the effective medium theory. Within this theory the different formulae expressing the refractive index can be employed (see Section 3.5). The Bruggeman formula is the most used one for this purpose. The Bruggeman formula enabling us to calculate the effective refractive index  $\hat{n}_{j,\text{ef}}$  of the fictitious thin film representing the microrough boundary between the  $(j - 1)$ -th and  $j$ -th film of the system exhibits the following form:

$$(1 - p_j) \frac{\hat{n}_{j-1}^2 - \hat{n}_{j,\text{ef}}^2}{\hat{n}_{j-1}^2 + 2\hat{n}_{j,\text{ef}}^2} + p_j \frac{\hat{n}_j^2 - \hat{n}_{j,\text{ef}}^2}{\hat{n}_j^2 + 2\hat{n}_{j,\text{ef}}^2} = 0, \quad (12)$$

where  $p_j$  is volume fraction of the  $j$ -th material in the fictitious film.

The isotropic and homogeneous fictitious films are not often suitable for approximation of the boundaries corresponding to MCRS. From the physical point of view it is reasonable to replace these rough boundaries by inhomogeneous fictitious film whose refractive index varies continuously along direction perpendicular to the boundaries of the film [5, 6] The optical quantities of these thin films are calculated using formulae known within the theory of inhomogeneous thin films (see below).

It should be noted that the theoretical approach presented above does not respect the scattering of light. Of course, in principle the influence of microroughness of the boundaries can be included using perturbation theories into the formulae expressing the optical quantities of the thin film systems (see the following section).

### 3.2 Slightly rough boundaries

The boundaries of the thin film system exhibiting the relations  $\sigma \ll \lambda$  and  $T \approx \lambda$  are called the slightly rough boundaries. For the thin film systems containing these boundaries it is necessary to use an approach corresponding to some perturbation theory if we want to express the formulae enabling us to calculate the optical quantities of these systems. To our knowledge the theory presented by Rice [7] belongs to the efficient perturbation theories allowing to derive the formulae usable for describing the slightly rough boundaries in a satisfactory way<sup>1</sup>.

Then the  $j$ -th slightly rough boundary taking place in the thin film system is described by the

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<sup>1</sup>This theory is known as the Rayleigh–Rice theory (RRT).

following matrix from the optical point of view:

$$\tilde{B}_{qj} = \frac{1}{\hat{t}_{qjR}} \begin{pmatrix} 1 & -\hat{r}_{qjL} \\ \hat{r}_{qjR} & \hat{t}_{qjR}\hat{t}_{qjL} - \hat{r}_{qjR}\hat{r}_{qjL} \end{pmatrix}, \quad (13)$$

where  $\hat{r}_{qjR}$ ,  $\hat{r}_{qjL}$ ,  $\hat{t}_{qjR}$  and  $\hat{t}_{qjL}$  are the Fresnel reflection and transmission coefficients of the  $j$ -th slightly rough boundary for the p- and s-polarizations. These Fresnel coefficients comprise the corrections expressing the influence of slight roughness and they can be calculated using the RRT [8]. The indices  $R$  and  $L$  distinguish the Fresnel coefficients corresponding to the waves incident on the boundary from the left side (right-going wave) and from the right side (left-going wave), respectively. Note that the matrix  $\tilde{B}_{qj}$  introduced in Eq. (3) represents the special form of this matrix  $\tilde{B}_{qj}$  written in Eq. (13) because for the smooth boundaries the following equations are true:  $\hat{t}_{qjR}\hat{t}_{qjL} - \hat{r}_{qjR}\hat{r}_{qjL} = 1$  and  $\hat{r}_{qjR} = -\hat{r}_{qjL}$ . If the adjacent boundaries to the  $j$ -th slightly rough boundary are sufficiently far from this boundary, i. e.  $d_{j-1} > T_j$  and  $d_j > T_j$ , one can use the same matrix formalism for expressing the optical quantities of thin film system containing the slightly rough boundaries as in the case of the system with the ideally smooth boundaries (see Section 2).

This matrix formalism can not be used for the rough systems containing one or more films for which the relations presented above are not fulfilled, i. e. it can not be used if the following relations are true for the  $j$ -th film:  $d_j < T_{j-1}$  and  $d_j < T_j$ . One can then employ a more complicated mathematical formalism for the expression of the transfer matrix  $\tilde{M}_{qj}$  representing the  $j$ -th film. In this case the formal expression of the transfer matrix  $\tilde{M}_{qj}$  is identical with the expression of the refraction matrix  $\tilde{B}_{qj}$  introduced in Eq. (13). Of course, the Fresnel coefficients existing in this transfer matrix correspond to the Fresnel coefficient of the slightly rough film that must be calculated using the RRT exactly (for detail see our earlier paper [9]). The foregoing fact is caused by the correlation of the electromagnetic field in the vicinity of the slightly rough boundaries. The correlation properties of this electromagnetic field was studied in our paper [10].

It should be pointed out that the calculations of the optical quantities of the thin film systems must be performed numerically within the RRT. This fact causes that the use of the approach based on RRT is a relatively very complicated (this statement is true for all the perturbation theories in general).

### 3.3 Inhomogeneity in refractive index

A profile of the complex refractive index across the thin film represent this inhomogeneity. The schematic diagram of  $j$ -th inhomogeneous film (IHF) of the system is plotted in Fig. 2. It is known that the solution of the Maxwell equations expressing the wave propagation within the inhomogeneous thin films gives the differential equations of the second order. In general these equations must be solved using numerical procedures. In spite of this fact one can derive the matrix formalism compatible with that presented above [11].

In this paper we shall deal with the solution corresponding to the approximation based on geometrical optics<sup>2</sup>. This approximation is acceptable if the gradient of  $\hat{n}(z)$  of the film is

<sup>2</sup>This approximation is known as Wentzel–Kramers–Brillouin–Jeffries (WKBJ) approximation.

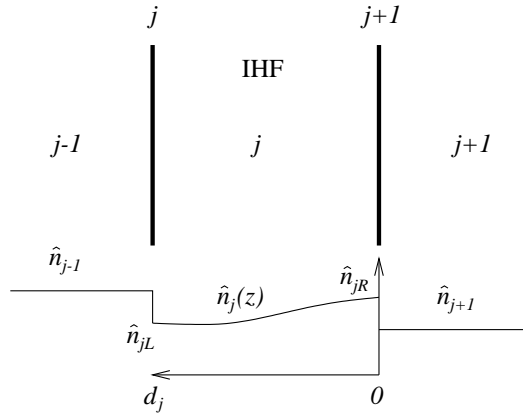


Fig. 2. Schematic diagram of the  $j$ -th inhomogeneous film of the isotropic thin film system.

relatively small [2]. Within the WKB approximation the phase matrix  $\tilde{T}_j$  must be replaced with the following matrix:

$$\tilde{T}_j = \begin{pmatrix} \hat{C}_j e^{i\hat{X}_j} & 0 \\ 0 & \hat{C}_j e^{-i\hat{X}_j} \end{pmatrix}, \quad (14)$$

where

$$\hat{C}_j = \sqrt[4]{\frac{\hat{n}_{jR}^2 - \sin^2 \theta_0}{\hat{n}_{jL}^2 - \sin^2 \theta_0}} \quad (15)$$

$$\hat{X}_j = \frac{2\pi}{\lambda} \int_0^{d_j} \sqrt{\hat{n}_j^2(z) - \sin^2 \theta_0} dz. \quad (16)$$

The symbols  $\hat{n}_{jL}$  and  $\hat{n}_{jR}$  represent the boundary values of the refractive index at the left and right boundaries of the  $j$ -th inhomogeneous thin film (see Fig. 2). The refraction matrices are formally identical with those corresponding to the homogeneous thin films. Of course, in the expressions of the Fresnel coefficients existing in these matrices the boundary values of the refractive indices of the films take place. If the profile of the refractive index of the  $j$ -th inhomogeneous thin film is chosen in the following way

$$\hat{n}_j^2(z) = \hat{n}_{jR}^2 + \frac{z}{d_j} (\hat{n}_{jL}^2 - \hat{n}_{jR}^2), \quad (17)$$

i. e. when the linear profile of the dielectric function is assumed, one can express the integral in Eqs. (16) as follows:

$$\hat{X}_j = \frac{4\pi}{3\lambda} d_j \frac{(\hat{n}_{jL}^2 - \sin^2 \theta_0)^{3/2} - (\hat{n}_{jR}^2 - \sin^2 \theta_0)^{3/2}}{\hat{n}_{jL}^2 - \hat{n}_{jR}^2}. \quad (18)$$

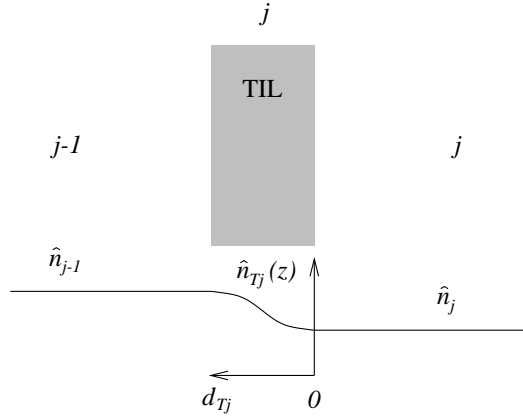


Fig. 3. Schematic diagram of the  $j$ -th boundary of the isotropic thin film system formed by transition interface layer.

One can thus see that for the refractive index profile expressed using Eq. (17) it is possible to include the influence of the inhomogeneous thin films into the expressions for the optical quantities of the thin film systems containing these films in an analytical way.

Note that in practice the inhomogeneous thin films are often replaced by corresponding multilayer systems at expressing the optical quantities of these films. This approximation can also be employed for the inhomogeneous thin films exhibiting relatively strong gradients in the refractive indices (see [1, 2]).

### 3.4 Transition interface layers

The boundaries taking place in the thin film systems are not often strictly sharp (i. e. these boundaries can not be represented by planes). This means that the boundaries mentioned can not be described by the refraction matrices  $\tilde{B}_{qj}$  presented above (see Eq. (3)). Such the boundaries are usually called the transition interface layers (TIL). From the physical point of view these TIL are represented by the inhomogeneous very thin film with a continuous profile of the refractive index. The boundary values of the refractive index of this TIL are equal to the values of the adjacent media (see Fig. 3).

Because the TIL are inhomogeneous thin films the matrix formalism used in the foregoing section can also be employed for the thin film system containing the TIL. From the mathematical point of view the situation concerning the TIL is simpler in comparison with the general inhomogeneous thin films since the values of the thicknesses  $d_T$  of the TIL are much smaller than the wavelength of incident light ( $d_T \ll \lambda$ ). This fact namely implies that the Drude approximation [1, 2, 12] can be employed for expressing the interaction of light with the TIL. Within this approximation it is possible to replace the refraction matrix  $\tilde{B}_{qj}$  introduced in Eq. (3) by the following matrix:

$$\tilde{B}_{qj} = \tilde{W}_{q(j-1)}^{-1} \tilde{X}_{qj} \tilde{W}_{qj}. \tag{19}$$

The matrices  $\tilde{W}_{qj}$  and  $\tilde{X}_{qj}$  are expressed as follows:

$$\tilde{W}_{sj} = \begin{pmatrix} 1 & 1 \\ i \frac{2\pi}{\lambda} \sqrt{\hat{n}_j^2 - \sin^2 \theta_0} & -i \frac{2\pi}{\lambda} \sqrt{\hat{n}_j^2 - \sin^2 \theta_0} \end{pmatrix}, \quad (20)$$

$$\tilde{W}_{pj} = \begin{pmatrix} \hat{n}_j & -\hat{n}_j \\ i \frac{2\pi}{\lambda \hat{n}_j} \sqrt{\hat{n}_j^2 - \sin^2 \theta_0} & i \frac{2\pi}{\lambda \hat{n}_j} \sqrt{\hat{n}_j^2 - \sin^2 \theta_0} \end{pmatrix}, \quad (21)$$

$$\tilde{X}_{sj} = \begin{pmatrix} 1 & d_{Tj} \\ d_{Tj} \left(\frac{2\pi}{\lambda}\right)^2 (\sin^2 \theta_0 - P) & 1 \end{pmatrix} \quad (22)$$

and

$$\tilde{X}_{pj} = \begin{pmatrix} 1 & d_{Tj}P \\ d_{Tj} \left(\frac{2\pi}{\lambda}\right)^2 (Q \sin^2 \theta_0 - 1) & 1 \end{pmatrix}, \quad (23)$$

where

$$P = \frac{1}{d_{Tj}} \int_0^{d_{Tj}} \hat{n}_{Tj}^2(z) dz, \quad Q = \frac{1}{d_{Tj}} \int_0^{d_{Tj}} \frac{1}{\hat{n}_{Tj}^2(z)} dz. \quad (24)$$

If the linear profile of the dielectric functions of the TIL is chosen, i. e.

$$\hat{n}_{Tj}^2(z) = \hat{n}_j^2 + \frac{z}{d_{Tj}} (\hat{n}_{j-1}^2 - \hat{n}_j^2), \quad (25)$$

one can calculate the integrals in Eqs. (24) in the following forms:

$$P = \frac{\hat{n}_j^2 + \hat{n}_{j-1}^2}{2}, \quad Q = \frac{\ln \hat{n}_j^2 - \ln \hat{n}_{j-1}^2}{\hat{n}_j^2 - \hat{n}_{j-1}^2}. \quad (26)$$

One can thus see that for the refractive index profile expressed using Eq. (25) it is possible to include the TIL into the expressions of the optical quantities of the thin film system containing these TIL in an analytical way.

It should be noted that in practice the TIL are often represented by the homogeneous very thin films with some “effective” refractive indices. In many cases this approximation is sufficient.

### 3.5 Volume inhomogeneity

Changes of the refractive index within the material of the thin film can be called volume inhomogeneity of this film from the optical point of view. It is very complicated to include this effect into the formulae expressing the optical quantities of the thin film systems. Only when the linear dimensions of the individual domains corresponding to the different values of refractive indices



inclusion	polarization	$q$
sphere	arbitrary	1/3
thin plate	perpendicular to plate	1
thin plate	parallel to plate	0
long cylinder	perpendicular to axis	1/2
long cylinder	parallel to axis	0

Table 1. Values of the depolarization factor  $q$  corresponding to the selected forms of the inclusions [13].

are much smaller than the wavelength of incident light one can use relatively simple mathematical procedures for taking into account of this inhomogeneity. In this case one can namely employ the theory of effective medium [4, 14]. Within this theory several formulae can be used. These formulae can be derived from the general “generic” formula which is written for a composite medium formed by two inclusions in the following way:

$$\frac{\hat{n}_{\text{ef}}^2 - \hat{n}_{\text{H}}^2}{\hat{n}_{\text{H}}^2 + q(\hat{n}_{\text{ef}}^2 - \hat{n}_{\text{H}}^2)} = p_{\text{A}} \frac{\hat{n}_{\text{A}}^2 - \hat{n}_{\text{H}}^2}{\hat{n}_{\text{H}}^2 + q(\hat{n}_{\text{A}}^2 - \hat{n}_{\text{H}}^2)} + p_{\text{B}} \frac{\hat{n}_{\text{B}}^2 - \hat{n}_{\text{H}}^2}{\hat{n}_{\text{H}}^2 + q(\hat{n}_{\text{B}}^2 - \hat{n}_{\text{H}}^2)}, \quad (27)$$

where  $\hat{n}_{\text{ef}}$ ,  $\hat{n}_{\text{A}}$ ,  $\hat{n}_{\text{B}}$  and  $\hat{n}_{\text{H}}$  denote the effective refractive index, the refractive index of the first material, the refractive index of the latter material and the refractive index of the host material, respectively. The symbols  $p_{\text{A}}$ ,  $p_{\text{B}}$  and  $q$  represent volume fraction of the first material, the latter material and the depolarization factor, respectively.

The values of the depolarization factor lays within the interval  $\langle 0, 1 \rangle$  and they depend on forms of the domains corresponding to the individual materials. For selected forms these values are summarized in Table 1.

If the domains are assumed in the spherical form ( $q = 1/3$ ) and the host medium is assumed to be formed by vacuum the generic formula implies the Lorentz–Lorenz formula, i. e.

$$\frac{\hat{n}_{\text{ef}}^2 - 1}{\hat{n}_{\text{ef}}^2 + 2} = p_{\text{A}} \frac{\hat{n}_{\text{A}}^2 - 1}{\hat{n}_{\text{A}}^2 + 2} + p_{\text{B}} \frac{\hat{n}_{\text{B}}^2 - 1}{\hat{n}_{\text{B}}^2 + 2}. \quad (28)$$

This Lorentz–Lorenz formula is suitable for inclusions A and B whose relative volumes within the host medium (vacuum) are small, i. e.  $p_{\text{A}} + p_{\text{B}} \ll 1$ . Therefore it is not reasonable to use this formula for describing the volume inhomogeneities in solids<sup>3</sup>.

If the spherical inclusions A are contained within the host medium formed by the material B the generic formula implies the Maxwell Garnett one [14], i. e.

$$\frac{\hat{n}_{\text{ef}}^2 - \hat{n}_{\text{B}}^2}{\hat{n}_{\text{ef}}^2 + 2\hat{n}_{\text{B}}^2} = p_{\text{A}} \frac{\hat{n}_{\text{A}}^2 - \hat{n}_{\text{B}}^2}{\hat{n}_{\text{A}}^2 + 2\hat{n}_{\text{B}}^2}. \quad (29)$$

This Maxwell Garnett formula is suitable for small relative volumes of the inclusions A in the host media B.

If in generic formula it is put that  $q = 1/3$ ,  $\hat{n}_{\text{H}} = \hat{n}_{\text{ef}}$  and  $p_{\text{A}} + p_{\text{B}} = 1$  one can obtain the Bruggeman formula [4], i. e.

$$p_{\text{A}} \frac{\hat{n}_{\text{A}}^2 - \hat{n}_{\text{ef}}^2}{\hat{n}_{\text{A}}^2 + 2\hat{n}_{\text{ef}}^2} + p_{\text{B}} \frac{\hat{n}_{\text{B}}^2 - \hat{n}_{\text{ef}}^2}{\hat{n}_{\text{B}}^2 + 2\hat{n}_{\text{ef}}^2} = 0. \quad (30)$$

<sup>3</sup>This formula is used to express the refractive indices of ion crystals in solid state physics.

Note that this Bruggeman formula is suitable for composite media exhibiting approximately identical relative volumes of both the materials A and B.

The other two special cases important from the practical point of view are generated from the general generic formula, i. e.

1. If  $q = 0$  then

$$\hat{n}_{\text{ef}}^2 = p_A \hat{n}_A^2 + p_B \hat{n}_B^2. \quad (31)$$

The foregoing equation corresponds to missing the depolarization effect. This situation sets in the special cases when the composite material is consisted of the inclusions formed by the long cylinders or thin plates and the polarization of the electric field is parallel to the axes of the cylinders or the plates, respectively (see Table 1).

2. If  $q = 1$  then

$$\frac{1}{\hat{n}_{\text{ef}}^2} = p_A \frac{1}{\hat{n}_A^2} + p_B \frac{1}{\hat{n}_B^2} \quad (32)$$

The foregoing equation corresponds to the strongest depolarization effect setting in the composite materials containing the inclusions formed by the thin plates in the case when the polarization of the electric field is perpendicular to the plates (see Table 1).

It is evident that all the foregoing equations can be generalized for the composite media comprising three and more inclusions.

Note that the matrix formalism presented for the ideal thin film systems can also be employed for the systems containing the thin films exhibiting the volume inhomogeneities. Of course, the refractive indices of the inhomogeneous thin films must be expressed by means of the formulae presented above.

#### 4 Example

In this section it will be introduced an illustration of using the foregoing matrix formalism. Let us assume that a sample of the thin film system originated in the following way. The smooth surface of silicon single crystal (c-Si) substrate is thermally oxidized. In this way the homogeneous  $\text{SiO}_2$  thin films with relatively sharp and smooth boundaries originates. Further by a plasma chemical vapor deposition procedure one can create a thin film of amorphous silicon (a-Si). It is known that this a-Si layer can exhibit a slightly rough upper boundary and certain transition interface layer at the lower boundary. Moreover, the a-Si layer can exhibit a certain profile of the refractive index.

This sample can be represented by the physical model plotted in Fig. 4. By applying the matrix formalism presented in this paper one is able to create the transfer matrix of this system as follows:

$$\tilde{M}_q = \tilde{B}_{q1} \tilde{T}_1 \tilde{B}_{q2} \tilde{T}_2 \tilde{B}_{q2}, \quad (33)$$

where the individual matrices have the following meaning:

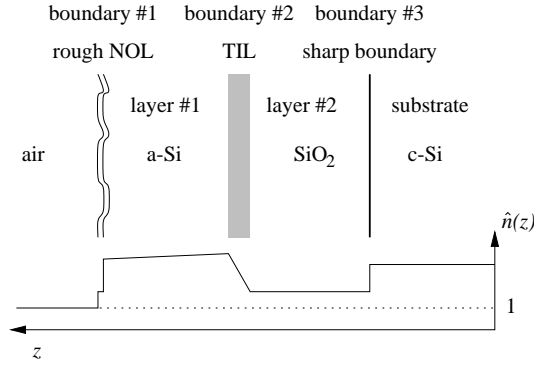


Fig. 4. Schematic diagram of the system formed by double layer a-Si/SiO<sub>2</sub> placed on the substrate formed by c-Si.

- The matrix  $\tilde{B}_{q1}$  represents the slightly rough native oxide layer (NOL) and it is given by Eq. (13). The Fresnel coefficients taking place in this matrix correspond to Fresnel coefficient of the rough NOL placed on a-Si.
- The matrix  $\tilde{T}_1$  corresponds to the inhomogeneous a-Si layer. This matrix can be expressed within the WKBJ approximation [see Eq. (14)].
- The matrix  $\tilde{B}_{q2}$  represents the TIL. It can be expressed using the Drude approximation. Then this matrix is given by the following matrix product:  $\tilde{B}_{q2} = \tilde{W}_{q1}^{-1} \tilde{X}_{q2} \tilde{W}_{q2}$  [see Eqs. (20)–(23)].
- The matrix  $\tilde{T}_2$  represents the homogeneous SiO<sub>2</sub> film [see Eq. (4)].
- The matrix  $\tilde{B}_{q3}$  corresponds to the sharp boundary between the SiO<sub>2</sub> film and c-Si substrate [see Eq. (3)].

## 5 Conclusion

In this paper the brief theoretical review of the influence of the important defects on the optical quantities of the thin film systems is performed. Thus the attention is devoted to the mathematical formalism enabling us to express the formulae for ellipsometric parameters, reflectances and transmittances of the system mentioned. It is shown that the uniform  $2 \times 2$  matrix formalism can be used for describing the optical properties of the thin film systems exhibiting the following defects:

- Microrough boundaries
- Slightly rough boundaries
- Inhomogeneity in refractive index
- Transition interface layers
- Volume inhomogeneity.

It should be pointed out that in practice the formulae for the the optical quantity mentioned were successfully used to analyze many thin films systems exhibiting the defects (e. g. [15–19]). Moreover, this  $2 \times 2$  matrix formalism can be extended to the  $4 \times 4$  matrix formalism employed for optically anisotropic thin film systems. This  $4 \times 4$  matrix is known as the Yeh's matrix formalism [20]

The more detailed description of the influence of the defects mentioned on the optical quantities of the thin film systems together with the experimental examples will be presented in our extended review paper [21]. In this paper the defects indescribable by the matrix formalism are discussed as well. These defects are moderate roughness and nonuniformity in thickness.

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### References

- [1] A. Vašíček: *Optics of Thin Films*, North-Holland, Amsterdam, 1960
- [2] Z. Knittl: *Optics of Thin Films*, Wiley, London, 1976
- [3] I. Ohlídal, K. Navrátil, M. Ohlídal: in *Progress in Optics XXXIV*, edited by E. Wolf, North-Holland, Amsterdam 1995, p. 249
- [4] D. A. G. Bruggeman: *Ann. Phys. (Leipzig)* **24** (1935) 636
- [5] L. Nevot, B. Pardo: *Rev. Phys. Appl.* **23** (1988) 1675
- [6] J. Szczyrbowski, K. Schmalzbauer, H. Hoffmann: *Thin Solid Films* **130** (1985) 57
- [7] S. O. Rice: *Commun. Pure Appl. Math.* **4** (1951) 351
- [8] R. Schiffer: *Appl. Opt.* **26** (1987) 704
- [9] D. Franta, I. Ohlídal: *J. Mod. Opt.* **45** (1998) 903
- [10] D. Franta, I. Ohlídal: *Opt. Commun.* **147** (1998) 349
- [11] R. Jacobson: in *Progress in Optics V*, edited by E. Wolf, North-Holland, Amsterdam, 1966, p. 249
- [12] P. Drude: *Wied. Ann.* **43** (1891) 136
- [13] C. Kittel: *Introduction to Solid State Physics*, Wiley, New York, 1976
- [14] J. C Maxwell Garnett: *Philos. Trans. R. Soc. London* **203** (1904) 385
- [15] I. Ohlídal, D. Franta, J. Hora, K. Navrátil, J. Weber, P. Janda: *Mikrochim. Acta (Suppl.)* **15** (1998) 177
- [16] I. Ohlídal, D. Franta, E. Pinčík, M. Ohlídal: *Surf. Interface Anal.* **28** (1999) 240
- [17] D. Franta, I. Ohlídal, D. Munzar, J. Hora, K. Navrátil, C. Manfredotti, F. Fizzotti, E. Vittone: *Thin Solid Films* **343–344** (1999) 295
- [18] D. Franta, I. Ohlídal, P. Klapetek: *Mikrochim. Acta* **132** (2000) 443
- [19] D. Franta, I. Ohlídal: *Surf. Interface Anal.* **29** (2000) in print
- [20] P. Yeh: *Surf. Sci.* **96** (1980) 41
- [21] I. Ohlídal, D. Franta: in *Progress in Optics XLI*, edited by E. Wolf, North-Holland, Amsterdam, 2000, in print