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Exact polynomial inversion for top transparent layer parameters on an arbitrary substrate in ellipsometry

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Abstract
We consider the inverse ellipsometric problem for a transparent layer on top of an isotropic substrate, which may consist of an arbitrary number of plane parallel homogeneous layers with complex refractive indexes, or have an arbitrary depth profile variation of the complex refractive index. It is shown that the task of finding the top layer parameters can be split into two. First, the top layer dielectric constant is determined by the roots of a fifth degree polynomial and then the layer thickness is found. Error propagation analysis is provided on a sample system and the stability of the method is estimated.

S Supplementary data are available from stacks.iop.org/JPhysCM/20/285225

1. Introduction

Ellipsometry is a precise noncontact and nondestructive method for investigation of the optical properties of different systems like bulk materials, thin films and multilayer structures. It is based on the detection of the change in the light polarization after interaction with a sample. Data treatment is based on a model that most closely describes the real system under investigation. When all the model parameters are known, the system optical response can usually be computed uniquely; this represents the forward ellipsometric task. More interesting however, is the inverse problem, where some system parameters (such as, for example, layer refractive index and thickness and/or refractive index depth profile) are considered as unknown, and have to be found from the experimentally measured ellipsometric quantities. Nonlinearity complicates the inverse problem considerably. In many cases a nonlinear minimization is the only choice. In such an approach [1], a suitably chosen measure of the experimental and model data misfit (a merit function) is minimized by varying the model parameters. Some general drawbacks are inherent to the nonlinear minimization, of which maybe the most critical is that it does not guarantee finding solutions in all situations. Usually the number of the solutions is not *a priori* known and the procedure may not find all the mathematical solutions corresponding to the global minima. This may be further complicated by the existence of local minima. As the solution of the inverse ellipsometric problem is usually not unique, it is very important to find all the mathematical solutions in order to select among them physically meaningful ones. As a consequence of the above, the minimization approach is not time deterministic, making it unsuitable for important ellipsometric applications such as real time parameter estimation and closed loop process control [2].

For some simple, but practically important systems, there are analytical solutions of the inverse ellipsometric problem: (1) a two-phase system with unknown complex refractive index of one of the phases [3]; (2) a single layer system with unknown layer thickness [3]; (3) a multilayer system with unknown thickness of any one of the layers [4]; (4) a single layer system with unknown complex refractive index of the substrate [5]; (5) a symmetric system of one layer of unknown thickness and real refractive index embedded in two identical phases having a real refractive index [6]. All these inversions lead to mathematical tasks of solving polynomials of a degree less than 5, and thus can be termed ‘analytical’.

In several other cases, the problem can also be reduced to a simpler task of finding the roots of a polynomial, but with a degree higher than 4. Although this is not an analytical

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solution, it has clear advantages over the standard minimization procedures. Finding the polynomial roots is well established numerical task and it gives all the possible solutions of the system [7]. The known polynomial solutions are: (6) an arbitrary multilayer system with unknown thicknesses of the any two layers [8]; (7) a one layer (3 phase) system with a uniform nonabsorbing [9] or an absorbing [10] substrate with unknown real refractive index and layer thickness.

In previous papers treating case (7) [9, 10], the fifth degree polynomials are derived using model dependent parameters (the Fresnel reflection coefficients for the boundary transparent layer/substrate). In this paper we consider a generalization of this case, using the generalized Fresnel reflection coefficients of the substrate in the incident medium. This effectively decouples the solution procedure from the model of the substrate structure, allowing the determination of the refractive index and thickness of a top transparent layer on an arbitrary substrate. This task has been discussed already, but in the thin layer limit [11]. Even for this approximate solution the polynomial degree is relatively high (8th order). Here we show that for this inverse ellipsometric problem the layer dielectric constant satisfies (exactly, in the frame of the given model) a fifth degree polynomial. Thus the initial task is split into two—first, finding the layer dielectric constant (or equivalently, the layer refractive index) as the roots of a 5th degree polynomial and second—the determination of the corresponding layer thickness.

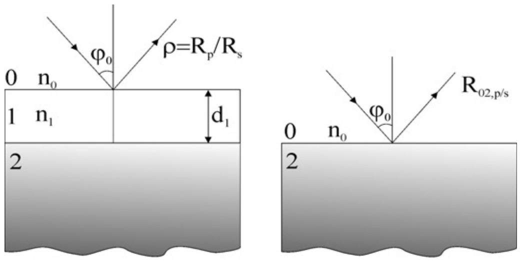
2. Derivation of the fifth degree polynomial

The system under consideration is a transparent top layer on a substrate consisting of an arbitrary number of plane parallel isotropic homogeneous layers with (generally) complex refractive indexes or, more generally, of a semi-infinite medium with an arbitrary plane parallel depth profile of the refractive index. The system is situated in a nonabsorbing ambient. The unknown parameters are the real refractive index and the thickness of the top layer. The above stated ellipsometric task is of great practical importance, for example when using ellipsometry for open or closed loop control in applications involving multiple layer deposition (optical coatings, filters), etching processes and others [2].

The optical response of such system is fully described by the complex amplitude reflection coefficients R_p and R_s for the two fundamental p- and s-linear polarizations. Conventional reflection ellipsometry gives partial information, determining the so called ellipsometric ratio ρ, or equivalently the two ellipsometric angles Ψ and Δ:

$$\rho = tg\Psi e^{i\Delta} = R_p/R_s. \tag{1}$$

Equation (1) connects the experimentally measured quantities Ψ and Δ with the optical system response—ratio of the reflection coefficients, which are functions of the system parameters. Further the indexes 0, 1 and 2 will be used for the ambient (refractive index n_0), the topmost layer (refractive index n_1 and thickness d_1, considered as unknown), and the underlying system respectively—figure 1(a).



(a) (b)

Figure 1. The structure under consideration with unknown top layer parameters (refractive index n_1 and thickness d_1)—(a). The underlying system is fully described by the generalized Fresnel coefficients ($R_{02,p/s}$) according to the ambient—(b).

The complex amplitude reflection coefficients R_p and R_s can be expressed by the top layer parameters and the underlying system optical response [12]:

$$R_{p/s} = \frac{r_{01p/s} + R_{12,p/s}Z}{1 + r_{01p/s}R_{12,p/s}Z}, \tag{2}$$

$$Z = \exp\left[-i\frac{4\pi d_1 n_1 \cos\varphi_1}{\lambda}\right], \tag{3}$$

$$r_{01p} = \frac{n_1\cos\varphi_0 - n_0\cos\varphi_1}{n_1\cos\varphi_0 + n_0\cos\varphi_1}, \tag{4}$$

$$r_{01s} = \frac{n_0\cos\varphi_0 - n_1\cos\varphi_1}{n_0\cos\varphi_0 + n_1\cos\varphi_1}, \tag{5}$$

where $r_{01p/s}$ are the Fresnel reflection coefficients at the boundary 0/1 and $R_{12,p/s}$ are the generalized Fresnel reflection coefficients at the boundary 1/2, λ is the wavelength and i is the imaginary unit. The angle of incidence φ_0 and the angle of refraction φ_1 (in the top layer) are connected by Snell's law: $n_0\sin\varphi_0 = n_1\sin\varphi_1$.

In equation (2) the unknown thickness appears only in the expression for Z, while all coefficients Z, $r_{01p/s}$ and $R_{12,p/s}$ depend on the unknown layer refractive index. In order to reduce the number of terms, which contain the unknown variables, it is convenient to express the generalized Fresnel coefficients ($R_{12,p/s}$) for the boundary unknown layer/underlying system by the reflection coefficients ($R_{02,p/s}$) of the underlying system according to the ambient—figure 1(b). In the case when the top layer thickness tends to zero (respectively $Z \to 1$), the reflection coefficients (2) of the system can be written as $R_{p/s} = R_{02,p/s}$. Then the coefficient $R_{12,p/s}$ can be expressed as:

$$R_{12,p/s} = \frac{R_{02,p/s} - r_{01p/s}}{1 - r_{01p/s}R_{02,p/s}}. \tag{6}$$

The coefficients $R_{02,p/s}$ are regarded further as known and the underlying system below the layer is fully described by them. This means that the presented solution of the inverse problem is applicable in the very general case of the underlying structure—the only requirement is that its scattering matrix is diagonal in the p/s presentation [3]. The coefficients $R_{02,p/s}$ can be computed easily by recursion, provided the underlying system parameters are known [13], or found from data treatment of previous ellipsometric measurements on the same system without the top layer. In the latter case, the procedure, described here, can be applied recursively for every next (transparent) top layer. The substitution of $R_{12,p/s}$ from equation (6) into (2) gives an expression for $R_{p/s}$, where the unknown parameters appear only in $r_{01p/s}$ and Z:

$$R_{p/s} = \frac{r_{01p/s}(1 - r_{01p/s}R_{02,p/s}) + (R_{02,p/s} - r_{01p/s})Z}{(1 - r_{01p/s}R_{02,p/s}) + r_{01p/s}(R_{02,p/s} - r_{01p/s})Z}. \quad (7)$$

To reduce further the number of terms containing the unknown refractive index, let us express the Fresnel coefficient r_{01p} through r_{01s} [14]:

$$r_{01p} = r_{01s}\frac{r_{01s} - \cos(2\varphi_0)}{1 - r_{01s}\cos(2\varphi_0)} = x\frac{x - c}{1 - xc}, \quad (8)$$

where for further brevity $c = \cos(2\varphi_0)$ and $x = r_{01s}$.

From (7) we obtain

$$R_s = \frac{x(1 - xA_s) + (A_s - x)Z}{(1 - xA_s) + x(A_s - x)Z}, \quad (9)$$

$$\begin{aligned} R_p = {} & \{x(x - c)[1 - xc - x(x - c)A_p] + [A_p(1 - xc) \\ & - x(x - c)](1 - xc)Z\}\{[1 - xc - x(x - c)A_p](1 - xc) \\ & + x(x - c)[A_p(1 - xc) - x(x - c)]Z\}^{-1}, \end{aligned} \quad (10)$$

where the substitutions $A_p = R_{02,p}$ and $A_s = R_{02,s}$ have been made.

Substituting the expressions for R_s and R_p from equations (9) and (10) into (1) results in a polynomial expression, in which the degree of x is six and of Z is two:

$$\begin{aligned} & a_{01}Zx^6 + (a_{12} + a_{11}Z + a_{10}Z^2)x^5 + (a_{22} + a_{21}Z + a_{20}Z^2)x^4 \\ & + (a_{30} + a_{31}Z + a_{30}Z^2)x^3 + (a_{20} + a_{21}Z + a_{22}Z^2)x^2 \\ & + (a_{10} + a_{11}Z + a_{12}Z^2)x + a_{01}Z = 0, \end{aligned} \quad (11)$$

where

$$\begin{aligned} a_{01} &= (A_p - \rho A_s); \\ a_{10} &= -(\rho + c); \\ a_{11} &= 2c(\rho A_s - A_p) - (1 + \rho c)A_sA_p + \rho + c; \\ a_{12} &= (1 + \rho c)A_sA_p; \\ a_{20} &= A_sc + c^2 + \rho A_s + 2\rho c - \rho A_pc + 1 - A_pc^2; \\ a_{21} &= A_pc^2 + A_p\rho A_s - 2\rho c + 2\rho A_pc + 2A_sA_pc - c^2 \\ & \quad + \rho A_sA_pc^2 - 1 - \rho A_sc^2 - 2A_sc; \qquad (12) \\ a_{22} &= \rho A_sc^2 - A_p\rho A_s - \rho A_sA_pc^2 + A_sc - 2A_sA_pc \\ & \quad - A_p - \rho A_pc; \\ a_{30} &= \rho A_pc^2 + A_p\rho - c - 2\rho A_sc + 2A_pc - \rho c^2 + \rho A_sA_pc \\ & \quad + A_sA_pc^2 - A_s - A_sc^2; \\ a_{31} &= 2A_s + 2\rho c^2 + 2c - 2A_sA_pc^2 - 2\rho A_pc^2 - 2\rho A_p \\ & \quad + 2A_sc^2 - 2\rho A_sA_pc. \end{aligned}$$

Equation (11) is a 6th degree polynomial of a real variable (x) with complex coefficients and along with its conjugated polynomial they both can be used to reduce the degree by eliminating any one of the polynomial terms. As the leading and the constant terms in (11) are the same, they both can be canceled simultaneously, thus reducing the resulting polynomial degree by 2. In the complex conjugated polynomial it is used that $Z^* = 1/Z$ (the symbol $*$ denotes complex conjugation), which holds true when n_0 and n_1 are real and the condition $n_1^2 > n_0^2\sin^2\varphi_0$ is satisfied. Finally this leads to a new polynomial in the form:

$$AZ^2 + BZ + C = 0, \quad (13)$$

where the coefficients A, B and C are all 4th degree polynomials of x:

$$\begin{aligned} A &= (a_{01}a_{12}^* - a_{01}^*a_{10})x^4 + (a_{01}a_{22}^* - a_{01}^*a_{20})x^3 \\ & \quad + (a_{01}a_{30}^* - a_{01}^*a_{30})x^2 + (a_{01}a_{20}^* - a_{01}^*a_{22})x \\ & \quad + a_{01}a_{10}^* - a_{01}^*a_{12} \\ B &= (a_{01}a_{11}^* - a_{01}^*a_{11})x^4 + (a_{01}a_{21}^* - a_{01}^*a_{21})x^3 \\ & \quad + (a_{01}a_{31}^* - a_{01}^*a_{31})x^2 + (a_{01}a_{21}^* - a_{01}^*a_{21})x \qquad (14) \\ & \quad + a_{01}a_{11}^* - a_{01}^*a_{11} \\ C &= (a_{01}a_{10}^* - a_{01}^*a_{12})x^4 + (a_{01}a_{20}^* - a_{01}^*a_{22})x^3 \\ & \quad + (a_{01}a_{30}^* - a_{01}^*a_{30})x^2 + (a_{01}a_{22}^* - a_{01}^*a_{20})x \\ & \quad + a_{01}a_{12}^* - a_{01}^*a_{10}. \end{aligned}$$

It can be shown that the identity $A + B + C = 0$, holds true for any value of x. This allows factorization of the equation (13):

$$(Z - 1)(AZ + A + B) = 0. \quad (15)$$

The factorization at this stage of the procedure simplifies the derivation of the polynomial, a step of which it has not been taken advantage in previous works [8, 9]. The solution $Z = 1$ of (15) corresponds to a special case when the layer thickness is equal to zero, or to a multiple thickness period $D_\varphi = \lambda/(2n_1\cos\varphi_1)$ and the layer refractive index is undeterminable. This situation is easily detectable, because when $Z = 1$, the measured quantity is $\rho = R_{02,p}/R_{02,s}$. Assuming that $Z \neq 1$ gives a linear equation for Z: $AZ + A + B = 0$. Using its conjugated expression and the fact that the coefficient B from (14) is pure imaginary, we obtain

$$Z = -A^*/A. \quad (16)$$

Equation (16) can be used for direct computation of the thickness if the corresponding layer refractive index is known.

Note that the coefficient A from (14) has a symmetric form:

$$A = a_1x^4 + b_1x^3 + c_1x^2 - b_1^*x - a_1^*, \quad (17)$$

where

$$\begin{aligned} a_1 &= a_{01}a_{12}^* - a_{01}^*a_{10}; \\ b_1 &= a_{01}a_{22}^* - a_{01}^*a_{20}; \\ c_1 &= a_{01}a_{30}^* - a_{01}^*a_{30}. \end{aligned} \quad (18)$$

Finally, by consecutive substitution of equations (16) and (17) in (9), we split the task and obtain an expression for R_s, which depends only on one unknown parameter (x). The resulting expression has a 6th degree polynomial in the numerator and the denominator. A common multiplier (x^2-1) can be canceled (assuming that $x^2 = r_{01s}^2 < 1$) and then

$$R_s = \frac{t_4x^4 + t_3x^3 + t_2x^2 + t_3x + t_4}{p_4x^4 + p_3x^3 + p_2x^2 + p_3x + p_4}, \tag{19}$$

where

$$\begin{aligned} t_2 &= b_1 + b_1^* - A_s(c_1 + a_1^* + a_1); \\ t_3 &= a_1 + a_1^* - A_s b_1; \\ t_4 &= -A_s a_1; \\ p_2 &= a_1 + a_1^* - c_1 - A_s(b_1 + b_1^*); \\ p_3 &= b_1^* - A_s(a_1 + a_1^*); \\ p_4 &= a_1^*. \end{aligned} \tag{20}$$

The same procedure can be applied by substitution of equation (16) in (10) and the final result is the ratio of two polynomials of 6th degree:

$$R_p = \frac{q_6x^6 + q_5x^5 + q_4x^4 + q_3x^3 + q_4x^2 + q_5x + q_6}{s_6x^6 + s_5x^5 + s_4x^4 + s_3x^3 + s_4x^2 + s_5x + s_6}, \tag{21}$$

where

$$\begin{aligned} q_3 &= (b_1 + b_1^*)(1 + c^2) - 2c(a_1 + a_1^*) - A_p[(b_1 + b_1^*)c^2 \\ &\quad + b_1 - b_1^* - 2ca_1 - 2c(c_1 + a_1^*)]; \\ q_4 &= (a_1 + a_1^*)(1 + c^2) - (b_1 + b_1^*)c - A_p[(a_1 + a_1^*)c^2 \\ &\quad + a_1 + c_1 - 2cb_1]; \\ q_5 &= -A_p(b_1 - 2ca_1) - c(a_1 + a_1^*); \\ q_6 &= -A_p a_1; \\ s_3 &= (b_1 + b_1^*)c^2 + 2c(c_1 - a_1 - a_1^*) + b_1^* - b_1 \\ &\quad + A_p[2c(a_1 + a_1^*) - (b_1 + b_1^*)(1 + c^2)]; \\ s_4 &= (a_1 + a_1^*)c^2 + a_1^* - c_1 - 2cb_1^* + A_p[(b_1 + b_1^*)c \\ &\quad - (a_1 + a_1^*)(1 + c^2)]; \\ s_5 &= A_p c(a_1 + a_1^*) - 2ca_1^* + b_1^*; \\ s_6 &= a_1^*. \end{aligned} \tag{22}$$

The numerators and denominators in the expressions for R_s, equation (19) and R_p, equation (21) are of even degree and have a symmetric form

$$\alpha_n x^n + \alpha_{n-1}x^{n-1} + \cdots + \alpha_{n/2}x^{n/2} + \cdots + \alpha_{n-1}x + \alpha_n = 0. \tag{23}$$

It can be shown that an nth degree polynomial of this kind can be recast as an $(n/2)$th degree polynomial of a new variable ($w = x + 1/x$), thus dividing the degree by two (see appendix). In our case

$$w = x + 1/x = 2(\varepsilon_1 + \varepsilon_0 \cos(2\varphi_0))/(\varepsilon_0 - \varepsilon_1), \tag{24}$$

where $\varepsilon_0 = n_0^2$ and $\varepsilon_1 = n_1^2$ are the ambient and the top layer dielectric constants, respectively. In terms of the new variable w the equations (19) and (21) take the form

$$R_s = \frac{t_4w^2 + t_3w + t_2 - 2t_4}{p_4w^2 + p_3x + p_2 - 2p_4}, \tag{25}$$

and

$$R_p = \frac{q_6w^3 + q_5w^2 + (q_4 - 3q_6)w + q_3 - 2q_5}{s_6w^3 + s_5w^2 + (s_4 - 3s_6)w + s_3 - 2s_5}, \tag{26}$$

where the polynomial coefficients are already defined in equations (20) and (22).

Finally, substituting (25) and (26) in (1) we obtain a 5th degree polynomial for w

$$m_5w^5 + m_4w^4 + m_3w^3 + m_2w^2 + m_1w + m_0 = 0, \tag{27}$$

with coefficients

$$\begin{aligned} m_0 &= \rho(t_2 - 2t_4)(s_3 - 2s_5) - (q_3 - 2q_5)(p_2 - 2p_4); \\ m_1 &= \rho[t_3(s_3 - 2s_5) + (t_2 - 2t_4)(s_4 - 3s_6)] \\ &\quad - (q_4 - 3q_6)(p_2 - 2p_4) - p_3(q_3 - 2q_5); \\ m_2 &= \rho[t_4(s_3 - 2s_5) + t_3(s_4 - 3s_6) + s_5(t_2 - 2t_4)] \\ &\quad - q_5(p_2 - 2p_4) - p_3(q_4 - 3q_6) - p_4(q_3 - 2q_5); \\ m_3 &= \rho[t_4(s_4 - 3s_6) + t_3s_5 + s_6(t_2 - 2t_4)] - q_6(p_2 - 2p_4) \\ &\quad - q_5p_3 - p_4(q_4 - 3q_6); \\ m_4 &= \rho(t_4s_5 + t_3s_6) - q_6p_3 - q_5p_4; \\ m_5 &= \rho t_4s_6 - q_6p_4. \end{aligned} \tag{28}$$

The five polynomial roots (27) give through equation (24) five mathematical solutions for the layer dielectric constant:

$$\varepsilon_1 = \varepsilon_0[w - 2\cos(2\varphi_0)]/(w + 2). \tag{29}$$

From this set of mathematical solutions complex solutions should be excluded, as they do not satisfy the initial assumptions.

The coefficients in (27), as derived above, are complex but for them the following relation holds:

$$\begin{aligned} m_l^*/m_l &= K, \qquad l = 0-5, \\ m_l &= 2\,\mathrm{Re}(m_l)/(1 + K), \end{aligned} \tag{30}$$

where K is a complex constant. The common complex multiplier $2/(1 + K)$ can be divided out, making (27) equivalent to a polynomial with real coefficients. Consequently, the number of physical solutions may be 5, 3 or 1, as the complex roots of (27) appear in conjugated pairs. For any physical solution the corresponding thickness can be computed from (3):

$$d_1 = \frac{\mathrm{i}\lambda \ln(Z)}{4\pi n_1 \cos\varphi_1} + \frac{k\lambda}{2n_1 \cos\varphi_1}, \tag{31}$$

where Z is determined from equations (16) and (17), k is an integer and the thickness is determined up to a multiple thickness period $D_\phi = \lambda/(2n_1 \cos\varphi_1)$ as usual for a transparent layer [3].

Table 1. Five polynomial solutions for the test. (Note: Simulation is for an angle of incidence 70°, wavelength 632.8 nm, system: dielectric layer ($n_1 = 1.49$, $d_1 = 50$)/silver layer ($n_2 = 0.06$–4.15i, $d_2 = 20$ nm)/glass substrate ($n_3 = 1.52$). The ellipsometric angles at these conditions are $\Psi = 42.0793$ and $\Delta = 79.0312$.)

Solution	Polynomial roots w equation (27)	Layer dielectric constant, ε_1	Layer refractive index, n_1	Layer thickness d_1 (nm)	Comment
1	−2.3835	2.2201	1.4900	50.0000	True solution
2	−1.4538	0.1433	0.3786	27.2516 + 183.9885i	Non-physical
3	−1.7141	−0.6366	0.7979i	11.0873	Non-physical
4	−1.9773 − 0.0447i	−3.2287 − 8.3169i	1.6871 − 2.4648i	3.0261 + 25.1677i	Non-mathematical
5	−1.9773 + 0.0447i	−3.2287 + 8.3169i	1.6871 + 2.4648i	−21.2200 − 13.8665i	Non-mathematical

As mentioned already, the above inversion procedure is a generalization of the polynomial solution for determination of the parameters of a transparent layer on top of a homogeneous semi-infinite substrate, which was described previously in [10]. Both solutions are equivalent in case of simple substrate.

3. Special case of reflection above the critical angle of the layer

For the special case when the index of the layer is lower than the index of the ambient media, the condition $n_1^2 > n_0^2 \sin^2 \varphi_0$ is not satisfied for angles of incidence greater than the critical angle of the 0/1 boundary. In this situation Z no longer has a modulus 1, but becomes real, in a contradiction with the initial assumption for the derivation of the polynomial. On the other side $x = r_{01s}$ becomes complex with modulus 1. The detailed calculations (not given here) shown that in this case the layer dielectric constant again satisfies the polynomial (27) with the same coefficients (28). This means that the determination of the layer dielectric constant (respectively the refractive index) can be treated uniquely using polynomial (27) in both cases.

For the determination of the layer thickness the equation (16) $Z = -A^*/A$ is no longer valid, but for the coefficients of A and B (14) the following relation holds true

$$a_k + b_k = a_k^*, \qquad k = 0 - 4. \tag{32}$$

Inserting (32) in (15), the expression for Z takes the form

$$Z = -\sum_k a_k^* x^k \Big/ \sum_k a_k x^k, \tag{33}$$

and the thickness is determined once again from equation (31).

4. Error propagation analysis

The polynomial inversion was tested on different multilayer structures using computer simulated data. The model considered here is a dielectric layer—metal layer—dielectric substrate system. The parameters were chosen as follows: ambient—air ($n_0 = 1$); top dielectric layer—$n_1 = 1.49$, $d_1 = 50$ nm; metal layer (Ag) $n_2 = 0.06$–4.15i [15], $d_2 = 20$ nm; substrate (glass) $n_3 = 1.52$ [16]. The values of the five solutions for the top layer dielectric constant along with their corresponding refractive indexes and thicknesses at angle of incidence 70° are given in table 1. Two of the polynomial roots appear as a complex conjugate couple and consequently can be rejected, as they do not satisfy the initial mathematical assumptions. The other three roots are real in the range from 0° to 90°. One of them (solution 3 from table 1) is negative and the corresponding refractive index is purely imaginary and can be rejected also. Solution (2) gives refractive index less than 1 and complex thickness and consequently can be rejected. Thus in this case, a unique solution (1 from table 1) can be selected from the set of the five mathematical solutions of the initial problem. It should be noted that this uniqueness is not warranted in every situation, then the selection of the correct root can be based on preliminary information, or by multiangle ellipsometric measurements.

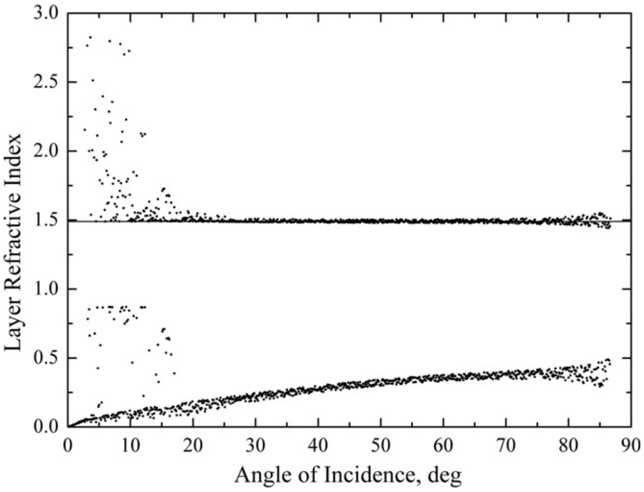


Figure 2. Scatter in refractive index values produced by the uniformly distributed error of 0.1° in Ψ and 0.2° in Δ for the described system. Solid line—the exact value. Upper curve corresponds to the physical solution.

To test the stability of the procedure on the described system, the ellipsometric angles (Ψ and Δ) were simulated in a wide range of incident angles from 0° to 90° at a wavelength 632.8 nm with a uniformly distributed error (0.1° in Ψ and 0.2° in Δ). These errors are much larger than the usually achievable accuracy of an ellipsometric device (0.01° in Ψ and 0.02° in Δ), but here they are chosen to demonstrate the stability of the solution. The refractive indexes of the two real roots are plotted on figure 2. The physical solution (1) is stable over the whole angle of incidence region, while the false root corresponding to solution (2) changes continuously from 0 (near 0°) to 0.5 (near 90°). The thickness corresponding to the lower refractive index (solution 2) is pure imaginary and

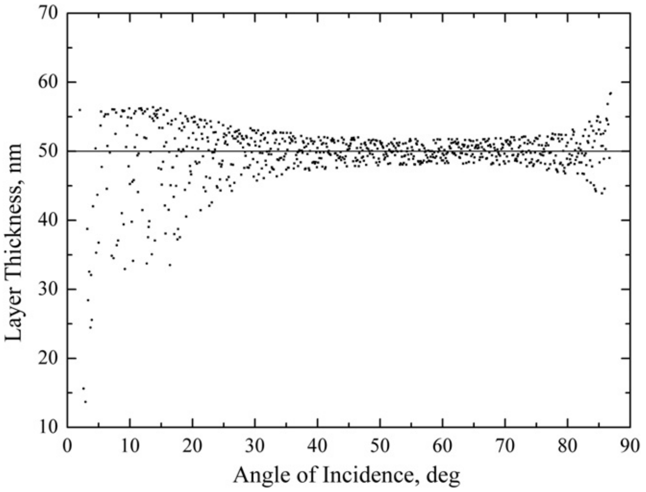


Figure 3. Scatter in the thickness values corresponding to the refractive index from figure 2 (upper curve). Solid line—the exact value. The thickness values, corresponding to the lower curve in figure 2 are complex.

the only one remaining is the true value (solution 1), shown on figure 3. The exact values of the layer parameters are also shown with solid lines on figures 2 and 3. The following features can be observed.

1. There is a large range of angles of incidence with a minimum error, where the deviation in refractive index is ±0.01 and in the thickness is ±2 nm.
2. The uniform spread of errors at low angles of incidence in the ellipsometric quantities Ψ and Δ causes a nonuniform spread in the layer parameters.
3. At angles of incidence near normal and oblique the scattering of the refractive index and layer thickness values are much larger than at the center of the region.

The stability of the solution was tested also in the case of smaller layer thickness (5 nm, or $d/\lambda = 0.008$). The errors introduced in the ellipsometric angles were chosen according to the usual accuracy of an ellipsometric device (0.01° in Ψ and 0.02° in Δ). The results show that at angle of incidence 70° at wavelength 632.8 nm the refractive index computed using the polynomial inversion procedure is 1.49 ± 0.05 and the thickness is 5.0 ± 0.2 nm.

Along with the stability of the algorithm, the error propagation analysis is useful for the determination of the optimal experimental conditions. Such a preliminary analysis should be performed on every particular model system under investigation. For example, in the above described situation at wavelength of 632.8 nm, an angle of incidence between 50° and 70° seems to be the best choice, as the deviation of the layer parameters from their exact values is minimal.

A computer program, written in Scilab (www.scilab.org), incorporating the above described method of the polynomial inversion for the parameters of a top transparent layer is provided in the supplementary material (available at stacks.iop.org/JPhysCM/20/285225).

5. Conclusion

In conclusion, for the first time we showed that the inverse ellipsometric problem for finding the layer refractive index and the thickness of a transparent layer on an arbitrary isotropic substrate could be split in two separate tasks. The first part of the problem is reduced to a fifth degree polynomial for the layer dielectric constant from which the corresponding thickness is computed. The polynomial inversion procedure gives all possible mathematical solutions, among which the physical one can be easily selected. Error propagation analysis demonstrates that the solution stability over small variations of the input data is good and the method can be successfully used for the determination of the top layer parameters.

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Appendix

Let us have a symmetric polynomial of even degree

$$\alpha_4 x^4 + \alpha_3 x^3 + \alpha_2 x^2 + \alpha_3 x + \alpha_4 = 0. \tag{A.1}$$

At $x \neq 0$ we can write:

$$x^2 \left[\alpha_4 \left(x^2 + \frac{1}{x^2} \right) + \alpha_3 \left(x + \frac{1}{x} \right) + \alpha_2 \right] = 0. \tag{A.2}$$

Using the substitutions;

$$\begin{gathered} w = x + 1/x, \\ x^2 + \frac{1}{x^2} = \left(x + \frac{1}{x} \right)^2 - 2 = w^2 - 2, \end{gathered} \tag{A.3}$$

in (A.2), the polynomial in the parenthesis is reduced to a second degree polynomial of w:

$$\alpha_4 w^2 + \alpha_3 w + \alpha_2 - 2\alpha_4 = 0. \tag{A.4}$$

The procedure is analogous for a sixth degree polynomial:

$$x^3 \left[\alpha_6 \left(x^3 + \frac{1}{x^3} \right) + \alpha_5 \left(x^2 + \frac{1}{x^2} \right) + \alpha_4 \left(x + \frac{1}{x} \right) + \alpha_3 \right] = 0. \tag{A.5}$$

Using the equations from (A.3) and

$$x^3 + \frac{1}{x^3} = \left(x + \frac{1}{x} \right)^3 - 3 \left(x + \frac{1}{x} \right) = w^3 - 3w, \tag{A.6}$$

the final form of the polynomial (A.5) in terms of the new variable w becomes

$$\alpha_6 w^3 + \alpha_5 w^2 + (\alpha_4 - 3\alpha_6) w + \alpha_3 - 2\alpha_5 = 0. \tag{A.7}$$

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