A GENERAL INVERSION METHOD
FOR SINGLE-WAVELENGTH ELLIPSOMETRY
OF SAMPLES WITH AN ARBITRARY NUMBER OF LAYERS

S. Bosch and F. Monzonís
Laboratori d'Òptica. Departament de Física Aplicada i Electrónica. Universitat de Barcelona
Diagonal 647, E-08028 Spain
Tel.: ++34 93 402 12 03
Fax: ++34 93 402 11 42

## 1. Introduction

A single-wavelength ellipsometric measurement is defined by means of two real quantities $\Delta$ ($0\leq\Delta\leq2\pi$) and $\Psi(0\leq\Psi\leq\pi/2)$ which are usually cast into a single complex value

$$\rho = \tan(\Psi)\exp(i\Delta).$$

The values $\Delta$ and $\Psi$ may be computed when the physical model and exact data describing the sample are perfectly known [1]. Conversely, assuming always we know the physical model, the knowledge of $\rho$ allows computing two of the real-valued parameters (refractive indices, extinction coefficients or thicknesses) defining the sample. In fact, in the most common case of layered structures, the last statement is not always true since the highly non-linear nature of the equations involved does not always guarantee the validity of inversion procedures. Besides, these have to be numerical ones [2][3][4], because only a very limited number of sample configurations allow the analytical inversion of the corresponding ellipsometric equations [5]. Anyway, the choice of the inversion procedure is always very important in order to guarantee the convergence in cases where the starting point for the iterations is quite far from the solution.

Within this context, focusing our attention in the single angle of incidence case, the reduction of dimensionality of the problem (whenever is possible) has proven to be a very useful technique. Namely, instead of iterating simultaneously for the two unknowns in our configuration (either refractive indices, absorption coefficients or thicknesses), much better convergence is obtained by iterating for only one of the unknowns, computing the other afterwards. This is the central idea of many existing algorithms, particularly the classical and most basic Reinberg method [2][3][4][5].

The conditions for the validity of the methods based on reduction of dimensionality are fulfilled for double layer samples provided one of the unknowns is one of the thicknesses [6]. This allows very

good convergence properties for double layer ellipsometric computations and the method is also valid for the most general case of two absorbing layers. The basis of the iteration method is solving the ellipsometric equation with respect to a complex exponential of the form

$$X \equiv \exp(-2i\beta), \quad \beta = 2\pi \, (d/\lambda) \, N \cos(\varphi) \qquad (1)$$

where d is the unknown thickness, N the complex refractive index of the layer and $\varphi$ the refraction angle within it (computable using Snell's law). This leads always to a quadratic equation with two complex roots $X_1$ and $X_2$, from which we may compute two thicknesses $d_1$ and $d_2$ using expression (1). Iterations have to tend to find a root whose associate thickness has no imaginary part [6].

Further insight into the previous ideas will lead to a general method for solving (by iteration) the ellipsometric equation corresponding to a layered structure composed by any number of layers which may be (all of them) absorbing. The method is developed for the single incidence angle case and the only restriction is that one of the two unknowns must be a thickness. The main advantage of the procedure is the very good convergence properties, independently of the number of layers composing the structure, since it leads always to a one dimension root finding algorithm.

## 2. Theory

The ellipsometric equation for reflection ellipsometry of layered structures may be formulated in different forms [7][8][9]. The most convenient procedure for our purposes is the matrix form, initially developed in [9], as expanded in [1]. We shall only present here the results we need for solving with respect to a thickness and another unknown.

Basically, there is a 2x2 matrix describing each layer and each interface. If n is the number of layers, the 'scattering matrix' S for the whole set is defined by

$$S = I_{0,1} \cdot L_1 \cdot I_{1,2} \cdot L_2 \cdots L_n \cdot I_{n,n+1}$$

$$L_j = \begin{pmatrix} \exp(i\beta_j) & 0 \\ 0 & \exp(-i\beta_j) \end{pmatrix}$$

**(2)**

$$\beta_j = \frac{2\pi}{\lambda} N_j d_j \cos(\phi_j)$$

$$I_{k,l} = \frac{1}{t_{k,l}} \begin{pmatrix} 1 & r_{k,l} \\ r_{k,l} & 1 \end{pmatrix}$$

where $r_{k,l}$ and $t_{k,l}$ are the corresponding Fresnel coefficients. In fact, we must consider two matrices $I_{k,l}$, one for each polarisation (p or s), leading to two final matrices S: $S^p$ and $S^s$. Thus, designing

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}, \tag{3}$$

we have, for reflection ellipsometry,

$$R_p = \frac{S^p_{21}}{S^p_{11}}, \; R_s = \frac{S^s_{21}}{S^s_{11}}$$

**(4)**

$$\rho \equiv \rho_r = \frac{R_p}{R_s}$$

If the only unknown in our structure is the thickness of layer j, we may express the product of all the outer matrices as a single matrix M and the product of the inner ones as a matrix N. This allows us to write S in terms of $L_j$ explicitly (either for p or s polarisation)

$$S = M.L_j.N$$

$$M = I_{0,1} \cdot L_1 \cdots L_{j\text{-}1} \cdot I_{j\text{-}1,j} \qquad \textbf{(5)}$$

$$N = I_{j,j+1} \cdot L_{j+1} \cdots L_n \cdot I_{n,n+1}$$

Calling X≡exp(iβ$_j$), this gives

$$S = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} . \begin{pmatrix} X & 0 \\ 0 & X^* \end{pmatrix} . \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix} \qquad \textbf{(6)}$$

and then

$$\rho = \frac{S^p_{21} S^s_{11}}{S^p_{11} S^s_{21}} = \frac{(M^p_{21} N^p_{11} X + M^p_{22} N^p_{21} X^*)(M^s_{11} N^s_{11} X + M^s_{12} N^s_{21} X^*)}{(M^p_{11} N^p_{11} X + M^p_{12} N^p_{21} X^*)(M^s_{21} N^s_{11} X + M^s_{22} N^s_{21} X^*)} \qquad \textbf{(7)}$$

which is

$$\begin{gathered}(M^p_{21} N^p_{11} M^s_{11} N^s_{11} - \rho M^s_{21} N^s_{11} M^p_{11} N^p_{11}) X^2 + (M^p_{22} N^p_{21} M^s_{12} N^s_{21} - \rho M^s_{22} N^s_{21} M^p_{12} N^p_{21})(X^*)^2 + \\ (M^p_{21} N^p_{11} M^s_{12} N^s_{21} + M^p_{22} N^p_{21} M^s_{11} N^s_{11} - \rho(M^s_{21} N^s_{11} M^p_{12} N^p_{21} + M^s_{22} N^s_{21} M^p_{11} N^p_{11}))X X^* = 0\end{gathered} \qquad \textbf{(8)}$$

Designing

$$\begin{aligned} a &= M^p_{21} N^p_{11} M^s_{11} N^s_{11} - \rho M^s_{21} N^s_{11} M^p_{11} N^p_{11} \\ b &= M^p_{22} N^p_{21} M^s_{12} N^s_{21} - \rho M^s_{22} N^s_{21} M^p_{12} N^p_{21} \\ c &= M^p_{21} N^p_{11} M^s_{12} N^s_{21} + M^p_{22} N^p_{21} M^s_{11} N^s_{11} - \rho(M^s_{21} N^s_{11} M^p_{12} N^p_{21} + M^s_{22} N^s_{21} M^p_{11} N^p_{11}) \end{aligned} \qquad \textbf{(9)}$$

equation (8) is

$$a X^2 + b(X^*)^2 + cX X^* = 0 \quad \textbf{(10)}$$

or

$$a\left(\frac{X}{X^*}\right)^2 + b\left(\frac{X}{X^*}\right) + c = 0 \quad \textbf{(11)}$$

This equation is very similar to our previous results for double layers [5][6], but not exactly the same since now $X=\exp(i\beta_j)$ and the last equation is quadratic in $X/X^*$, not in X.

Thus, if the only unknown in our general multilayer configuration is the thickness $d_j$ of one of layer j and we have one ellipsometric measurement ρ, the thickness may be computed from the last equation in $X/X^*$.

**3. Numerical solving procedures**

Comparing the final equations just obtained for the n-layer case with the previous formulations for double layer samples [5][6], we may expect that all the techniques already developped can be appropriate for the present n-layer situation.

In fact, taking into account equation (11) and the results of [5], one may immediately devise an iteration method to solve it. As stated above, we will have two unknowns: one is thickness $d_j$ an the other one any of the remaining physical parameters. Using the measured value ρ and an approximate value for the other parameter (say t), we may compute a, b and c in (11). Solving this equation we may find $Z \equiv X/X^*$ for the assumed value t (we really have two roots $Z_1$ and $Z_2$). Since t will not be the exact (searched) value, neither $Z_1$ nor $Z_2$ will actually be unit modulus complex numbers. Thus, we may iterate to find the right value t, which is the one giving a root Z with $|Z|=1$. Once we have Z, we may compute X and $d_j$.

The procedure just proposed is valid to find the physical solution; the problem is that it also finds non-physical (only mathematical) solutions when layer j is absorbing. To demonstrate this point we have to note we are only iterating to find a complex number $Z=r.\exp(i\theta)$ with $|Z|=r=1$. If layer j is transparent, $k_j=0$ and $N_j=n_j$, so $\beta_j$ is real and $Z=\exp(2i\beta_j)$, giving for the thickness the real number

$$d_j = \frac{-i\lambda \log Z}{4\pi\, n_j \cos(\phi_j)} \qquad \textbf{(12)}$$

(the determinations of the 'log' correspond to the different thickness cycles). If layer j is not transparent, $|Z|=r=1$ does not guarantee that any value

$$d_j = \frac{-i\lambda \log Z}{4\pi\, N_j \cos(\phi_j)} \qquad \textbf{(13)}$$

is a real number.

To avoid all these non-physical solutions we have to use a more subtle iteration procedure, as the one proposed in [6]. For each value of the iteration parameter t, we do not only compute Z but also X, and the order of the 'log' giving the smaller imaginary part to $d_j$. This will give the right iteration procedure.

Therefore, depending on the distinctive fact of solving for the thickness of a layer which is transparent or absorbing, we may develop algorithms based on equating to 1 the modulus of the roots of (11) or on equating to 0 the imaginary part of the thickness computed from the roots. As the second possibility is more general than the first, in which follows we shall only consider in detail how to minimize for the imaginary part of the thickness. Similar procedures would be useful for the modulus of the roots.

To illustrate the details, let us suppose we are looking for the thickness $d_j$ of layer j and the real part of the refractive index $n_m$ of layer m, with all the remaining parameters known. We will use an upper and a lower limit for $n_m$ ($n_m'$ and $n_m''$) which should be as close as possible to the solution. Taking any of these two index values (say $n_m'$) and using the measured $(\Delta,\Psi)$, the coefficients a, b and c in equation (11&&) are determined and Z is directly computable. In fact, as Z is a complex value coming from a quadratic equation, there are actually two roots for each refractive index; for each root Z using (13&) we get $d_j$. The multiple solutions are

$$d_M = d_0 + M \frac{\lambda}{2\, N_j \cos(\phi_j)}, \quad M = integer \qquad \textbf{(14)}$$

where

$$d_0 = \frac{i\lambda \ln(r) - \lambda\theta}{4\pi N_j \cos(\phi_j)} \quad \textbf{(15)}$$

If $k_j$=0 ($N_j \equiv n_j$, j is a transparent layer), the term $\lambda/\{2\ n_j \cos(\varphi_j)\}$ is the well known thickness cycle; otherwise one has to keep track of several low M-order solutions. To be precise, physically meaningful solutions should come from values M giving no imaginary part to $d_M$ (and positive real part also). The right value of M might not be very high, because the second term in (&&) increases linearly with M while the first term is constant. Thus, one has to keep track of several low M-orders only, choosing the one giving thicknesses with the smaller imaginary part. In this way, from each Z we select a single value $d_M$ for the thickness of layer j. Moreover, among the two roots arising from $n_m'$ as a guess for $n_m$, we choose the one whose corresponding thickness (called $d_j'$) has the smaller imaginary part. Thus, finally, only two different values $d_j'$ and $d_j''$ (from $n_m'$ and $n_m''$ respectively) are algebraically deduced from (14&) and (15&) after our initial bracketing of the unknown index $n_m$. The most common situation is

$$\mathrm{Im}(d_j') < 0 < \mathrm{Im}(d_j'') \quad \text{or} \quad \mathrm{Im}(d_j') > 0 > \mathrm{Im}(d_j'') \qquad (16)$$

since the correct index value must give $\mathrm{Im}(d_j') = 0$ . Deviation from this assumption is only dependent on the accuracy of the index guess. Assuming that one of the two conditions (16&) holds, a straight-forward numerical problem remains: starting from two values $n_m'$ and $n_m''$ of the independent variable which bracket a root of the function $\mathrm{Im}(d_j)$, one has to find the root $n_m$ and the corresponding complex value $d_j$ . In computer programs, either a simple bisection method or the more efficient Brent algorithm may be used for root finding [10]. Obvious modifications will solve the other cases: iterating for $k_m$ or $d_m$.

## 4. Adressing practical issues by means of a graphical procedure

The analysis of convergence properties, precision, accuracy and error propagation in the proposed method may always be easily done by implementing a straightforward graphical representation of the procedure. Exactly as in [5] and [6], the present tecniques allow a useful graphical implementation. Since the iteration methods are based on approaching to zero the imaginary parts of pairs of complex numbers derived from a quadratic equation, the graphical development is based on plotting the imaginary parts of the two quantities we get for each value of the iteration variable. This variable may be any of the configuration parameters. The solutions are the roots of the curves.

By plotting the curves for a wide range of the iteration variable, the convergence of any

numerical algorithm for root finding is absolutely obviated. In fact, the graphical procedures guarantee the convergence of our numerical method when a solution exists and it may also reveal other unexpected solutions [6].

Regarding the precision, accuracy and error propagation in the inversion procedure, we should note, first of all, that there is no overdetermination of the unknowns, since from the pair of real quantities ($\Delta$,$\Psi$) we look for two real values. Thus, there is only a small uncertainty in the computed values due to numerical truncation and limiting tolerances in the solving algorithms. In practice, the main source of error is the imprecision in the values $\Delta$, $\Psi$, $\varphi$, optical constants of the substrate and other 'known' values. Although theoretical developments on error propagation have been established (see for example Ref. 8), a simple and safe way of testing our results is just recalculate them for the estimated limiting values $\Delta \pm \delta\Delta$, $\Psi \pm \delta\Psi$, $\varphi \pm \delta\varphi$, etc., as illustrated in the following example.

Let us consider an ideal sample (sketched in fig.1) consisting of a silicon wafer covered by three layers, whose relevant data are (for $\lambda$=6328 A): $n_1$=1.460, $k_1$=0.000, $d_1$=20 A, $n_2$=3.870, $k_2$=0.037, $d_2$=5000 A, $n_3$=1.460, $k_3$=0.000, $d_3$=200 A, and $n_4$=3.858, $k_4$=0.018 (substrate). When measured at 70 deg., the corresponding values are $\Delta$=145.446 and $\Psi$=14.094 . This kind of sample is common in the electronic industry. Suppose we know $\Delta$, $\Psi$, and all the physical data of this sample, except the thickness ($d_2$) and refractive index ($n_2$) of the intermediate polysilicon layer. Figure 2 plots...(one of the branches only) (order 6 is the wright one...)

Assuming $\delta\Delta$= and $\delta\Psi$= and considering the plus/minus possibilities we obtain figure 3... We see we can still identify the right order for this level of uncertainity in $\Delta$ and $\Psi$)..., provided we already estimate our ref index to be in the range nmin, nmax... In fact, it also helps having an idea of the unknown thickness, because the roots shown in figure 2 are...(llista), so our order is...

Similar considerations could be analyzed starting from figure 4, where we show the results equivalent to fig. 2, but when solving for $k_2$ and $d_2$.

## 5. Conclusions

We have developped a general mathematical formulation and closely related numerical procedures for solving the ellipsometric equation of a substrate covered by an arbitrary (but known) number of transparent or absorbing layers. From a single measurement ($\Delta$,$\Psi$), the procedure allows finding any two-parameter combination, provided one of the unknowns is a thickness.

**REFERENCES.**

[1] R.M.A. Azzam and N.M. Bashara, in: Ellipsometry and polarized light (North-Holland Publ. Amsterdam, 1977), ch. 4.

[2] A.R. Reinberg. Appl. Opt. 11 (1972) 1273.

[3] S.S. So. Surf. Sci. 56 (1976) 97.

[4] T. Easwarakhanthan, C. Michel and S. Ravelet. Surf. Sci. 197 (1988) 339.

[5] S. Bosch. Surf. Sci. 289 (1993) 411.

[6] S. Bosch and F. Monzonís. Surf. Sci. accepted.

[7] A. Vasicek, *Optics of Thin Films*, North-Holland, New York, 1960.

[8] F. Abelès, Ann. de Physique, 5 (1950) 596.

[9] P.C.S. Hayfield and G.W.T. White, in E. Passaglia, R.R. Stromberg and J. Kruger (eds.), *Ellipsometry in the Measurement of Surfaces and Thin Films*, Natl. Bur. Std. Misc. Publ. 256, US Government Printing Office, Washington, DC, 1964, p. 157.

[10] W.H. Press, B.P. Flannery, S.A. Teukolsky and W.T. Wetterling, in: Numerical Recipes in C (Cambridge University Press, Cambridge, 1988), ch. 9.