TECHNICAL NOTE

Numerical algorithm for spectroscopic ellipsometry of thick transparent films

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We present a numerical method for spectroscopic ellipsometry of thick transparent films. When an analytical expression for the dispersion of the refractive index (which contains several unknown coefficients) is assumed, the procedure is based on fitting the coefficients at a fixed thickness. Then the thickness is varied within a range (according to its approximate value). The final result given by our method is as follows: The sample thickness is considered to be the one that gives the best fitting. The refractive index is defined by the coefficients obtained for this thickness. © 1998 Optical Society of America

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1. Introduction

Ellipsometry is a standard characterization technique for thin-film manufacture because of its intrinsic high sensitivity and its nondestructive nature. One of the particular applications in which ellipsometry provides the best accuracy is in the study of very thin films. In this case, spectrophotometric methods are not useful since there are no interference extrema in the transmittance or the reflectance spectra. Conversely, for relatively thick films (several wavelengths of the considered working range) the use of ellipsometric methods is less widespread because they face several drawbacks, making spectrophotometry the most common practice.

Recently, an interesting study of the characterization of thick transparent films by variable-angle spectroscopic ellipsometry has been published.[1] In this study, the specific problems related to the thickness of the layer have been revised. One of the topics implicated in this study is the numerical methods that have been used for the inversion of the measured ellipsometric data. In fact, the detailed treatment of this problem is not presented in the text, but its significance in the characterization of the thick layers is evident.

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Let us analyze Figs. 2 and 3 of Ref. 1. To illustrate the model calculation proposed, the authors consider a theoretical spectrum of the Δ, Ψ angles corresponding to a 9-μm layer on a silicon substrate. They assume that the optical properties of the layer are given by the Cauchy model

$$n(\lambda) = A + B/\lambda^2 + C/\lambda^4 \quad (1)$$

with the values $A = 1.5364$, $B = 5.564 \times 10^{+3}$ nm^2, and $C = 8.010 \times 10^{+4}$ nm^4. The spectrum is calculated for an angle of incidence of 70° in the 500–850 wavelength region. It is explained in the text in Ref. 1 that the plots of χ^2 versus thickness were obtained with "a series of least squares minimizations to find the coefficients (A, B, C), with the thickness fixed for each minimization." In the particular case of Fig. 2, various χ^2 minima are obtained, and there is no doubt of the identification of the right thickness since the correct one has a noticeably lower value for χ^2 than the wrong ones. In the case of working with simulated data having a small amount of statistic noise added, a plot like Fig. 3 is obtained. The authors note here that the minima are now closer together and the values of χ^2 at the valleys are similar. It is evident that the existence of these side minima is an important drawback for the proposed method, because it leads to the requirement of a previous determination of the thickness range of the layer by profilometer measurements.

Our aim is to propose a numerical method for the inversion of the ellipsometric data that does not lead to the existence of side spurious minima. The method is simple, easy to be implemented numerically, and shows good convergence properties when tested with simulated data having statistical noise added.

2. Method

In its most basic implementation, the method that we present comprises the two following steps:

1. Perform the ellipsometric data inversion (assuming a fixed thickness) by use of a monochromatic algorithm to find (n, k) for each wavelength independently.
2. Use a best-fitting algorithm for the data (n, k) obtained in the previous step to determine the constants that define the dispersion model adopted. Compute the χ^2 that corresponds to the best fitting.

These two steps allow for the computation of χ^2 for the thickness assumed in step 1. Repeating the process for a set of thicknesses within a variation range, one gets a plot χ^2 versus layer thickness. We will show that this procedure does not lead to spurious minima and also that it is very stable against noise in the data.

Let us explain in more detail the two steps. Step 1 is a repeated application of any single-layer monochromatic ellipsometry algorithm that determines (n, k) at a known thickness from the ellipsometric data (Δ, Ψ), for example, a two-dimensional simplex on the variables (n, k).[2] Approximate values for the unknowns are needed to start any monochromatic algorithm, but it is important to note that these must be supplied only for one starting wavelength λ_0 since the result (n, k) for one wavelength may be the approximate value for the next one (as it is always quite close, say 10 nm apart). In our particular case we must supply an approximate value for the refractive index n_{approx} at one of the wavelengths (λ_0) of the range of measurements. Since our method assumes a fixed thickness for step 2, inverting $\Delta(\lambda_0)$ and $\Psi(\lambda_0)$ will generate $n(\lambda_0)$ and $k(\lambda_0)$. Note that in the case of computed ellipsometric data corresponding to an ideal transparent layer we will have $k \equiv 0$, but for noisy data, k will be small but nonzero (the values may increase with noise). For the next wavelength, say λ_1, we may use $n(\lambda_0)$ instead of n_{approx}, repeating the monochromatic algorithm. For real ellipsometric data, we expect a behavior for $k(\lambda)$ similar to the noisy case. Thus at the end of step 2, we have the full spectrum $n(\lambda)$ and $k(\lambda)$ at a fixed layer thickness for the wavelength range considered.

Step 2 consists of applying a best-fitting algorithm to the spectrum obtained in step 1. Thus we need to assume a dispersion formula, fit the coefficients of this formula, and calculate the final merit function. This merit function may be the χ^2 estimator, but it could also be any other measure of the deviation between data and model. In our implementation of the method, the dispersion formula is the one shown above and the best-fitting procedure used is the singular value decomposition.[3]

Regarding the repetition of the process, to obtain the plot of χ^2 versus layer thickness, it is evident that this is the most simple version of a one-dimensional minimization algorithm. The limits of the thickness range, and the step for increments defines the number of times that steps 1 and 2 will be performed and also the accuracy in the final thickness determination.

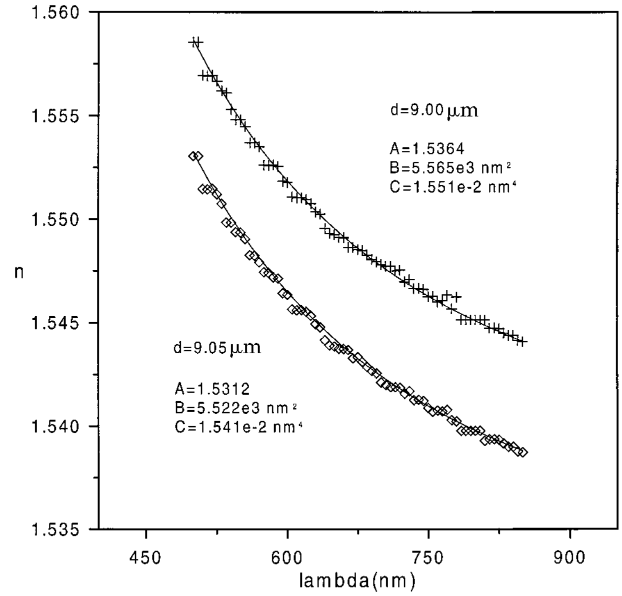

Fig. 1. Refractive-index values and best fittings to the Cauchy model corresponding to assumed thicknesses, 9.0 and 9.05 μm, for the data with $\sigma = 1.0°$ noise added.

3. Results

To illustrate the performances of our numerical procedure, we have applied it to the same theoretical spectrum of Figs. 2 and 3 in Ref. 1, but with different levels of statistical noise added to the ellipsometric data. We start by computing the spectroscopic (Δ, Ψ) values corresponding to an ideal sample consisting of a perfect 9-μm-thick layer on a semi-infinite silicon substrate. Three cases have been considered: exact (Δ, Ψ) data, and data with both $\sigma = 0.3°$ and $1.0°$ rms noise added. The previously described method has been applied to the three sets of theoretical spectra, when thicknesses from 8.7 to 9.3 μm were considered.

Figure 1 shows two sets of refractive-index values and their best fittings to the Cauchy model [Eq. (1)] by singular value decomposition corresponding to two assumed thicknesses, 9.0 and 9.05 μm, for the data with $\sigma = 1.0°$ noise added. As explained in the description of step 1, the use of the result for one wavelength as the starting point for the next one in the SIMPLEX algorithm guarantees the continuity in the values of the refractive index and, consequently, the smoothness of the subsequent fitting. A problem could appear in the vicinity of the singular points related to the thickness cycle of transparent layers, i.e., when thickness (d), refractive index (n), wave-

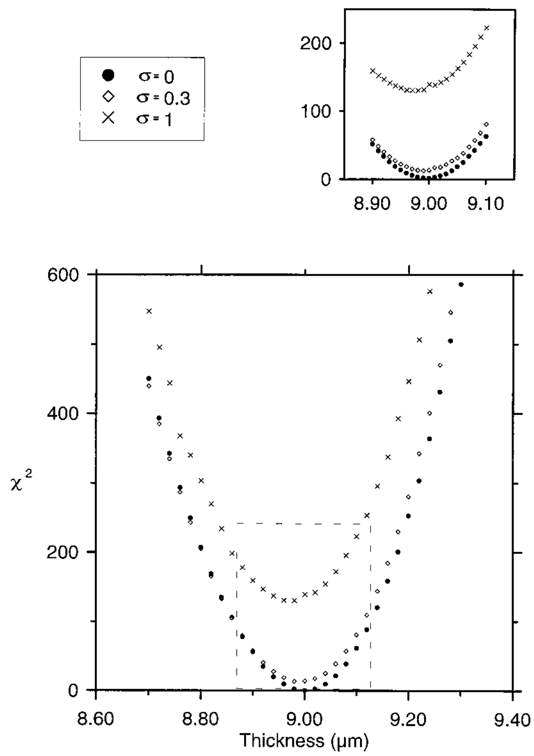

Fig. 2. Plots of χ^2 versus layer thickness for three data sets corresponding to noise levels $\sigma = 0°, 0.3°, 1.0°$.

length (λ), and incidence angle (ϕ) fulfill the expression

$$d = \frac{m\lambda}{2\sqrt{n^2 - \sin^2 \phi}} \quad m = 0, 1, 2 \tag{2}$$

since one may obtain a meaningless value of n for noisy data. It is unlikely to meet the conditions leading to Eq. (2) however, but even in this case it is easy to protect the point-by-point reinitialization of the SIMPLEX algorithm against misleading values of n by considering the starting value for the initialization to be more than one wavelength, that is, by looking at the last two or three n values found and not allowing variations that are too large.

Figure 2 plots χ^2 versus layer thickness for three sets of data having $\sigma = 0°$, 0.3°, and 1.0° noise added. The interval between thicknesses is 20 nm for the full range and 10 nm in the inset for the zone near the minimum.

From the figure we note that the method proposed works quite well, giving only one minima for all the noise levels considered. One may note that there is a small but noticeable displacement of the absolute minimum with respect to the 9-μm value. This is due to the noise introduced in the data that may generate statistic fluctuations that become more important as the noise level increases.

In conclusion, the numerical method proposed eliminates some of the drawbacks of the ellipsometric data analysis developed in Ref. 1 for thick layers.

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