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Inverse problem solving and optical index determination of resist films by ellipsometry

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A R T I C L E  I N F O

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Spectroscopic ellipsometry (SE) is known to be a technique of great sensitivity in thickness determination of thin layers. The sensitivity is said to be close to some angstrom when optical indexes of materials are perfectly known. However, for resist films, those optical indexes are unknown and can vary from one process to another. Optical indexes and film thicknesses are determined by using Fresnel laws in order to calculate theoretical ellipsometry signatures and by solving the inverse problem. This article presents two strategies developed by LTM in order to accurately determine optical indexes and the thickness of resist films.

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1. Introduction

In microelectronics ellipsometry is a widely used technique to determine film thickness. The principle of this technique is to measure the change of polarization of a light beam as it is reflected from a flat surface. Theory of ellipsometry is detailed in the Handbook of Tompkins and Irene [1]. The measured parameter is the Fresnel ratio \( \rho \) defined as:

\[
\rho = \frac{\sin^2 \theta}{\sin^2 \theta_N}
\]

where \( \psi \) and \( \Delta \) are ellipsometry angles. Since no direct measurement of the sample’s optical properties is achieved accuracy is linked to an inverse problem solving. The basis of the inverse problem solving requires to know the sample structure, i.e. the number of layer, the order of magnitude of the layers thickness and of the optical indexes of the materials. In this study, the sample structure is a single layer with optical indexes \( (n, k) \) and thickness \( e \) coating a flat substrate of known optical indexes (silicon). The thickness of the substrate is supposed infinite (true for an absorbing substrate). By using Fresnel laws, theoretical values of \( \psi \) and \( \Delta \) are calculated with initial guess values of \( (n, k) \) and \( e \). Minimizing the errors between the measured values and the theoretical ones allows the determination of \( e \) and \( (n, k) \). The difficulty of solving the inverse problem is due to the fact that the number of unknown parameters equals or is greater than the number of measured parameters. For instance, two values of \( \psi \) and \( \Delta \) are measured while three unknowns parameters \( (n, k \) and \( e) \) must be determined at each wavelength. Such under deterministic system may give strongly correlated values of the parameters. Hence, the number of measured parameters must be increased or the number of unknown ones must be reduced. One solution is to use spectroscopic measurements and to assume that \( n \) and \( k \) are linked to the wavelength of the light through dispersion laws. For instance a transparent Cauchy dispersion law decreases the number of unknown parameters from \( 2N + 1 \) to \( 3 + 1 \) (the 1 being the value of \( e) \), \( N \) being the wavelength sampling number of a scan. Finally films thicknesses are determined accurately if a transparent range is suitable to describe the optical indexes variation of the material. However, for absorbing materials, optical indexes are not accurately determined for the whole spectral range as, often, dispersion laws are too simple to describe the optical properties of the film. Moreover, for very thin films thickness error is not acceptable (2–5 nm for 10–20 nm thick films). Hilfiker et al. [2] gives a survey of several methods to reduce the correlation between the unknown parameters (here between the thickness and optical constants) of thin absorbing films. Among these methods are multiple sample analysis, interference enhancement, multiple angle measurements, multiple ambient analysis, Kramers–Kronig relations and so on. Several experimental results are given to confirm the theoretical settings. Bobro et al. [3] study an ill-posed inverse ellipsometric problem in order to obtain stable solutions. The problem is solved with the help of multi-angle measurements for ultra thin films. The authors announce that they successfully studied films with thickness ranging from 2 to 10 nm. Rosa [4] also study an inverse problem of ellipsometry for thin films in order to determine the thickness, the refractive index and the extinction coefficient. A statistical method is used in order to determine the solution and the standard errors. For inhomogeneous films, Tonova...
and Konova [5] propose an algorithm to obtain the refractive index and the thickness of the material. Once again, multiple incidence angle measurements are used. Djurisic et al. [6] use reflectance $R$ and transmittance $T$ measurements to compute $(n, k)$ and the film thickness. They use acceptance-probability-controlled simulated annealing algorithm with adaptive move generation procedure to determine unknown parameters. Flammich et al. [7] describe a method to determine optical constants from single angle reflection $R$ and transmittance $T$ measurements. In this approach the layer thickness is simultaneously determined with optical constants, ensuring the continuity of the refractive index as a function of wavelength. Often, ellipsometer tools are set to a single angle, especially for the monitoring of etching processes. Determining precisely $n$ and $k$ for single angle system is then mandatory if very accurate thickness measurements are needed. This study explains how to precisely determine $n$ and $k$ of an unknown material with measurements done at one measurement angle. Two strategies were developed by LTM, one assuming that $n$ and $k$ follow complex dispersion laws (up to five absorption peaks) and the second one with the Tikhonov regularization on the $(n, k)$ values. Both methods will be compared. Solutions that allow accurate measurements of $n$ and $k$ with one angle measurements will be suggested.

2. Experimental procedure

The ellipsometer used for this study is a phase modulated spectroscopic ellipsometer purchased from Horiba Jobin Yvon. Measurements are achieved in the energy range 1.5–6.5 eV. Incident angle is set to 70°. Angles position of the analyzer and modulator
are 45° and 0°, respectively. Here the measured parameters are \( I_s \) and \( I_c \) and are linked to \( w \) and \( D \) through:

\[
I_s = \sin(2w) \sin(D)
\]

\[
I_c = \sin(2w) \cos(D)
\]

Measured samples are two resist films 144 nm and 297.5 nm thick. The studied resist is a commercial E-Beam resist from Sumitomo (NEB22).

Two strategies were developed in order to determine film thickness and optical indexes. The first one consists in using the Lorentz oscillator model that describes the complex dielectric permittivity \( \varepsilon \) of the resist as a sum of Lorentz peaks,

\[
\varepsilon = \varepsilon_{\infty} + \frac{(\varepsilon_i - \varepsilon_{\infty}) E_t^2}{E_t^2 - E^2 + i\gamma E} + \sum_{j=1}^{N} \frac{f_j E_{0j}^2}{E_{0j}^2 - E^2 + i\gamma_j E}
\]

(1)

\( \varepsilon_{\infty} \) and \( \varepsilon_i \) being respectively the dielectric permittivity for infinite and zero energies, \( E_t \) is the energy centring the gap jump oscillator and \( I_t \) the half width at maximum. The last term of Eq. (1) is a sum of weaker oscillators centered at energies \( E_{0j} \) with half width at maximum \( \gamma_j \) and strength \( f_j \). This model is well suited to describe dielectric materials. The optical indexes are calculated by using the relation which links \( \varepsilon, n \) and \( k \): \( (n - ik)^2 = \varepsilon \).

Knowing \( \varepsilon, n \) and \( k \), a theoretical ellipsometry signature is obtained using Fresnel laws. The total number \( N \) of extra peaks is set to five. The algorithm developed for this study first evaluates the film thickness by using a Cauchy dispersion law. After this initial thickness determination, \( n \) and \( k \) are determined by adding one by one the peaks. Once an optimal solution is found for one peak.
(by minimizing the error between the experimental and the theoretical data), the next peak is added. In such an optimization strategy, the local minimum will freeze the $n$ and $k$ determination far from the real solution. To avoid this, multiple initial conditions are used. The best one will give the solution closest to the reality. Initial peak position will not be chosen randomly, it will be set at energy values, where the error between the experimental and theoretical data are the greatest. Finally, parameters are not free to move in an infinity range. Lower and upper bounds will be used. Once $n$ and $k$ simulated values are very close to reality, the last step of the algorithm consists in allowing unbounded parameters variations. This strategy allows determining accurately most of the resist optical indexes, but, for some cases the local minimum cannot be avoided. However the great advantage to this model is that the final $n$ and $k$ will verify Kramers–Kronig relations. It means that the final $n$ and $k$ have a physical meaning.

In the second strategy, the principle is a point by point optimization. In order to avoid erroneous results due to measurement noise or local minimum, regularization is used. Here one does not need to use any initial dispersion law but inputs a proper initial guess of the optical indexes $n$ and $k$. The aim is to obtain smoothed parameter curves using a regularization technique called Tikhonov regularization [8]. Inverse problem solving consists in minimizing a cost function. Eq. (2) expresses the optimal solution of the problem.

$$x^* = \arg \min_x \{ |F(x) - b|^2 + \beta^2 |x|^2 \}$$

The first term consists in minimizing the gap between the experimental data $b$ and the theoretically computed function $F$ with
unknown $x$ (here $x = (n, k)$). The second term is the regularization function that allows to constraint the variation of the $x$ using the second order derivatives (Hessian matrix $L$ is used in the computation). The parameter $\beta$ is used in the regularization process as a smoothing parameter. In order to determine the best $\beta$ we use a cross-validation technique. The best $\beta$ gives the lowest errors compared to the others. For more details on this technique see our [9]. However, as for any inverse problem resolution, initial conditions greatly impact on the accuracy of the final solution. Hence, the Tikhonov regularization will be applied to the solution obtained by the first strategy which gives a good guess of these initial conditions.

3. Results and discussion

Firstly the thicker resist film was studied. The thickness was determined by a Cauchy fit of the spectra in the 1.5–3.5 eV range. The result gives a thickness of 297.5 nm. Once the thickness is known, both previously detailed strategies are applied in order to obtain the optical index of the NEB22 resist. Fig. 1 shows the optical index $n$ and $k$ determined by the multiple Lorentz oscillator model and by the Tikhonov regularization. One can see that both strategies give almost the same $n$ and $k$. Three main absorption peaks are observed. Fig. 2 shows the residual errors after the inverse problem solving. Errors due to the multiple oscillator modelling are quite scattered and are locally not acceptable (above 5 times natural noise of the signal represented by the two horizontal lines). One the other hand, Tikhonov regularization gives the lowest errors. As no real difference appears on the $n$ and $k$ spectra obtained by those two techniques, we can postulate that ellipsometry is sensitive to small changes of optical indexes.

Then the thinner film is studied. The measured thickness of the film is 144 nm. Fig. 3 shows the $n$ and $k$ obtained by the two methods for the thin NEB22 film. Here again both strategies give almost similar results, except in the UV range between 6 and 6.5 eV where two curves can be observed. Surprisingly, Fig. 4 shows low residual errors for the multiple oscillator strategy and for the Tikhonov regularization, even in the 6–6.5 eV range. However, Tikhonov regularization gives the lowest residual between the experimental data and the theoretical signature. Hence, Tikhonov regularization seems to be the appropriate method in order to precisely determine optical indexes of unknown materials. Fig. 5 shows the variation of $n$ and $k$ with the energy of the light for the NEB22 obtained with the Tikhonov regularization for the two films. Some differences are visible for energies above 5.5 eV. As NEB22 is composed mainly of low molecular weight macromolecules, no real impact on the physical properties is expected in such a range of thickness. In fact the observed differences are artefacts of the inverse problem solving. The optical index determination by ellipsometry should be done with great care as different solutions might be obtained for the same material.

Finally, both ellisometric spectra will be used at once in order to determine $n$ and $k$ of the material. As it is considered that $n$ and $k$ remain unchanged for the 297.5 nm and the 144 nm thick film, both spectra should be correctly fitted. Fig. 6 shows the final results on the $n$ and $k$ values obtained by both methods. One can see that slight differences between the two solutions are observed for energies higher than 5.5 eV. Fig. 7 shows the residual error obtained by both methods and the Tikhonov regularization is once again the best method. The low values of the residue point out that the two NEB22 films have the same optical properties. The advantage of using two thicknesses is that the final solution is forced to meet a physical meaning (no other solution would fit both spectra). Therefore, by using a single angle ellipsometer it is possible to accurately determine optical indexes by using two samples of different thickness. Of course this can be applied to multi thickness studies, so that the final solution will be very robust and independent of measurements noises. Moreover, this will also be a way to detect bad calibrations range of ellipsometers. Those bad calibration zones will be located where the residual error values are unacceptable with respect to the measurements noise.

4. Conclusion

Two inverse problem solving strategies were used in order to determine the optical indexes of a resist with the best possible accuracy. The first one consists in using a complex dispersion law of oscillators whose position, width and strength were optimized in order to fit experimental curves. The second one consists in using an optimized regularization parameter (Tikhonov) with
initial conditions close to the reality. Both methods give robust results. However, the regularization method seems to be more accurate. Optical indexes of NEB22 were precisely determined in the 1.5–5.5 eV range and were properly estimated in the 5.5–6.5 eV range.

In order to increase the accuracy of the $n$ and $k$ determination, multiple spectra were fitted at once in order to minimize the impact of measurement noise or imperfect calibration. Once again, Tikhonov regularization is the best solution in order to determine the optical properties. Nevertheless, calibration accuracy may have a non negligible impact on local values of $n$ and $k$ when the residual error is highest than the natural noise of the measurement.

References