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Optimal Calibration for Rotating Analyzer Ellipsometer

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We have modeled most errors, which affect the measurement accuracy, with Jone's matrix. From the simulation, we can characterize the errors and take good aids for selecting components and designing ellipsometer. The traditional residual method has good performance when there are only azimuth angle errors and extinction errors, but it has not good performance when there are other errors. We have proposed the optimal calibration method for overcoming the residual method. The optimal method selects error values to have the least square difference between the measured thickness and the simulated thickness. We can reduce the design variables to three, incident angle error, and azimuth angle errors of polarizer and analyzer. The optimization results are slightly different from the residual method, and have smaller standard deviation of errors than the residual method. The experiment shows good agreement with the simulations.

Key Words : Ellipsometer, Optimal Calibration

1. Introduction

It is well known that the ellipsometric method is the most accurate optical way to study reflecting surfaces (the measurement of the optical constants of a material or thin-layer parameters). However, it makes use of optical and mechanical components that are always prone to induce more or less important errors (imperfect polarizers, azimuth angle error, etc.). In addition, the alignment relative to the incident and reflected light beams, always delicate, must not be altered by the rotation of some of the optical components. Moreover, all ellipsometric methods must have an adjustment of the azimuth angle of the polarizers with respect to the plane of incidence [Fig. 1]. If this adjustment is not accurate, a systematic error appears in the ellipsometric measurements. Several publications and scientific books have dealt with these subjects (Dignam and Moskovits, 1970 ; Aspnes and Studna, 1971 ; 1975 ; Adams and Bashara, 1976 ; Collins, 1990 ; Azzam and Bashara, 1977). This alignment of azimuth angle is called as calibration.

Calibration procedures for rotating analyzer ellipsometers were first described in detail by van der Meulen and Hien (1974) and by Aspnes

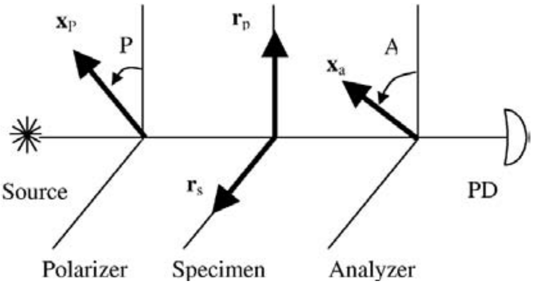

Fig. 1 Alignment for azimuth angle

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(1990) in 1974. Both methods are similar, relying on the fact that a light wave reflected from the surface of any isotropic sample is linearly polarized if the incident wave is linearly polarized in the *p* or *s* directions. Aspnes's method is more powerful in that it explicitly includes first-order corrections to the calibration values caused by optical activity of the polarizer and analyzer prisms.

2. Modeling of Errors

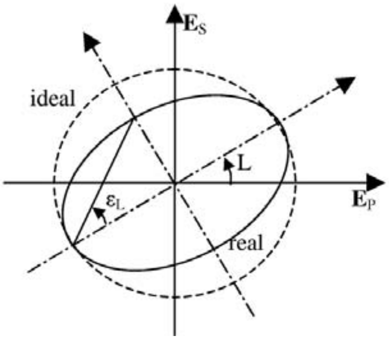
2.1 Light source

2.1.1 Polarization error

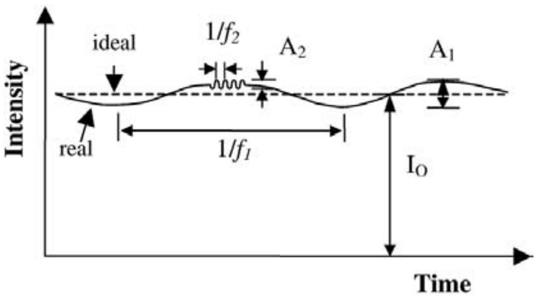
The ideal light source has a circular polarization state which is the dashed line in Fig. 2(a). However, the real light source has elliptic polarization state which is the continuous line in Fig. 2(a).

$$R(L)\,T_L=\begin{bmatrix}\cos L & -\sin L\\ \sin L & \cos L\end{bmatrix}\begin{bmatrix}\cos\varepsilon_L\\ i\sin\varepsilon_L\end{bmatrix}I_C \qquad (1)$$

which describes a polarization state whose amplitude I_C, azimuth L and ellipticity angle ε_L.



(a) Polarization



(b) Fluctuation

Fig. 2 Modeling for light source' errors

2.1.2 Fluctuation error

The amplitude is not exactly constant but fluctuates and drifts with time in Fig. 2(b). The fluctuation consists of two different frequencies; one is very low, the other is very high with respect to measurement frequency. Since ellipsometer measures not intensities but the ratios of intensities, low frequency fluctuation (f_1), drift, is canceled out. Since ellipsometer uses the Fourier analysis, the high frequency fluctuation (f_2) or random noises are averaged and cannot affect the measured results.

$$I_C(t)=I_O+A_1\sin(2\pi f_1 t)+A_2 rand(t) \qquad (2)$$

2.1.3 Wavelength error

Wavelength of light source may change to several nanometers. HeNe Laser is very stable source, but the laser diode may change to several nanometers due to both temperature drift and random noises. Wavelength error significantly affects measurement and analysis of specimen, but the wavelength is hardly changed.

$$\lambda(t)=\lambda_O+A_1\sin(2\pi f_1 t+A_2 rand(t)) \qquad (3)$$

2.2 Polarizer and analyzer

2.2.1 Extinction error and azimuth angle error

Linear polarizers are rotated at polarizer and analyzer. The ideal linear polarizer gives a prefect linear polarization state, but real linear polarizer has an extinction error which gives slightly

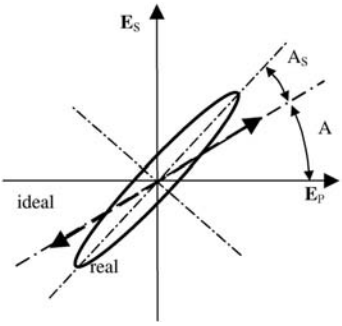


Fig. 3 Modeling for polarizer and analyzer's errors

elliptic polarization state (Fig. 3). The azimuth angle error with respect to the plane of incidence occurs when the linear polarizer is misaligned at motor, and the motor is driven with the time delay of electric circuit.

$$R(-A+A_e)\begin{bmatrix}1 & 0\\ 0 & ie_A\end{bmatrix}R(A-A_e) \tag{4}$$

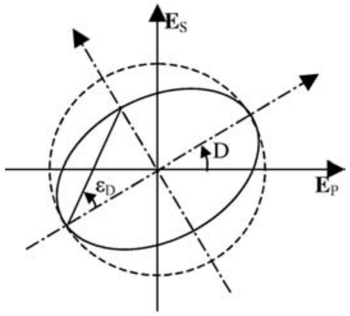
where A is azimuth angle, A_e azimuth angle error, and e_A extinction ratio. The same equation applies for polarizer.

2.3 Detector

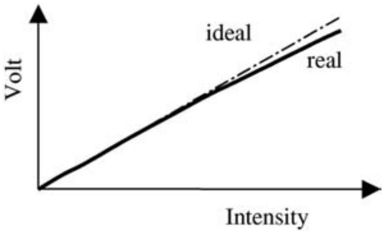
2.3.1 Polarization dependence error

Detector converts intensity to volt. The ideal detector should not depend on the polarization state but depend on only the intensity of entering light. Figure 4(a) shows both ideal and real detector. The real detector converts the intensities to the different volts according to the polarization state of entering light.

$$T_D R(D)=\begin{bmatrix}1 & 0\\ 0 & \tan\varepsilon_D\end{bmatrix}R(D) \tag{5}$$



(a) Polarization dependence



(b) Nonlinearity

Fig. 4 Modeling for detector's errors

where D is the azimuth angle of polarization and ε_D the angle of ellipticity.

2.3.2 Nonlinearity error

The ideal detector has the linear proportion of volts to intensities, but the real detector has the nonlinear proportion. Figure 4(b) shows both linear and nonlinear characteristics. The modeling for the nonlinear characteristics follows

$$V=C_0+I+C_2I^2 \tag{6}$$

where C_0 and C_2 are coefficients, and I intensity, and V volt.

2.3.3 Fluctuation error

The detector has fluctuation errors which arise from the electric circuit or the interface with computer. These noises are random errors, and these may be canceled out by averaging or low-pass filters. The fluctuation errors are inserted to the C_0 in Eq. (6).

$$C_0(t)=C_0^0+D_1\sin(2\pi q_1 t)+D_2\,rand(t) \tag{7}$$

2.4 Frame and environments

2.4.1 Incident angle error

The accuracy for the angle of incidence is determined by the manufacturing accuracy or motor's resolution for variable incident angle. When there is no process for alignment of sample, the angle of incidence may be altered by putting new specimen on the stage. Since the incident angle is directly related to the ellipsometric parameters, the incident angle error should be compensated.

$$\theta=\theta_0+\delta\theta \tag{8}$$

2.4.2 Mechanical vibration error

Since the mechanical vibrations alter the optical light paths, the measured intensities vary along to mechanical vibrations. When the frequency of the vibrations is proportional to the frequency of the measurement, the vibration will affect the measurement. If not, the vibrations may be canceled out by averaging or Fourier analysis. The random noises can be inserted into the 3rd term of Eq. (7).

2.4.3 Outer lights

Outer lights are the all lights except for light source. If the frequency of fluctuation for outer lights is proportional to the frequency of measurement, the outer lights may affect the measurement. If not, the outer lights may be canceled out by averaging or Fourier analysis. It can be also inserted into the 3rd term of Eq. (7).

3. Analysis of Errors

We simulate effects of the each error on the measurement for the purpose of understanding the characteristics of the each error. We can effectively use this analysis datum to purchase the ellipsometric components and to design the ellipsometer. We can also use these analysis datum to calibrate the manufactured ellipsometer systematically.

The simulation conditions are as follows. The polarizer is held at a fixed azimuth angle P=45° and the wavelength of light source is 650 nm at incident angle 70°, and the specimen is Air-SiO_2-Si where the complex refractive indexes are $N_{SiO2}=1.45654$ and $N_{Si}=3.85010-i0.01639$. The thickness of the film SiO_2 changes from 30 nm to about 600 nm. The sampling number of the analyzer is 1000 points per revolution.

We have already modeled each error in the previous chapter. The resulted electric field on the detector is expressed by the Jones matrix and calculus

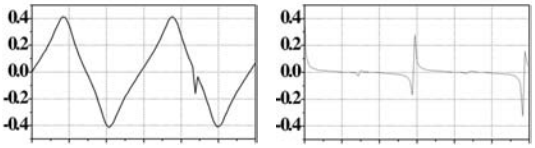
$$\begin{aligned} E_D = T_D R(D) R(-A+A_e) T_A R(A-A_e) \\ T_S R(-P+P_e) T_P R(P-P_e) R(L) T_L \end{aligned} \tag{9}$$

The other errors, which are not inserted in above equation, are inserted in the Eq. (7).

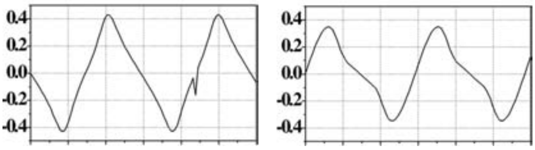
Figure 5 shows the thickness errors according to the film thickness. A careful look for the Figure 5 tells that there are some jumps near about 147, 292, 440, 587 nm. A reason is the periodic thickness. The ellipsometric parameters periodically change according to the thickness of film. Small disturbances of ellipsometric parameter can cause the large disturbance of thickness around periodic or half periodic thickness of specimen. Therefore, we can neglect these abrupt jumps.

The extinction error of polarizer is more sensitive than analyzer, and is more effective about 80 nm than below 10 nm. However, the extinction error of analyzer is more effective below 10 nm than at others. The azimuth angle error of polarizer is also more sensitive than analyzer, and is more sensitive at other thickness than below 10 nm. Figure 5(c)-(d) show that the errors between each other are symmetric about zero value.

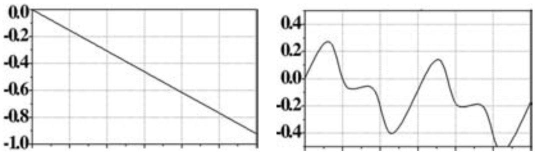
(a) Extinction Error of Polarizer 3.0E-3 (b) Extinction Error of Analyzer 1.0E-2



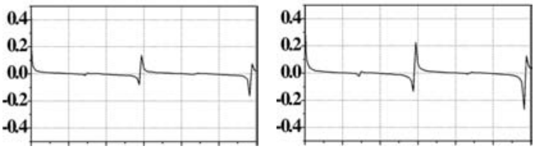
(c) Azimuth Angle Error of Polarizer 0.18 deg (d) Azimuth Angle Error of Analyzer 0.36 deg



(e) Wavelength Error of Light source 1 nm (f) Incident Angle Error 0.1 deg



(g) Nonlinearity Error of Detector −0.0003 (h) Bias Error of Detector 0.0001 Volt



(i) Ellipticity Angle Error of Detector 0.02 deg (j) Random Noises 1%

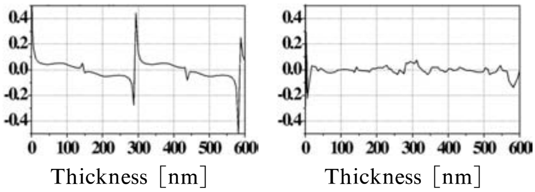


Fig. 5 Simulated thickness errors when the ellipsometer has the specified errors

The wavelength error of light source is more effective at larger thickness. The thickness errors linearly depend on the thickness of the film. The incident angle error is also more effective at larger thickness, but the errors are not linear. The nonlinearity error and bias error of detector is mainly sensitive at the very thin films, below 1 nm, but those errors are not effective at thick films. The random noises include all noises such as the electric fluctuation, light source fluctuation, mechanical vibration, and outer lights etc. The random noises are also very sensitive at the thin film, especially below 1 nm, but those errors are not effective at thick film.

From the simulation, we can know that the errors of detector are very effective only at very thin film, below 1 nm. Though the extinction error of analyzer is also effective at very thin film, the thickness errors is not large. The extinction error of polarizer and azimuth angle errors of both polarizer and analyzer are periodically effective, and these errors are fortunately not effective at very thin film. The incident angle error and wavelength error of light source are more effective at thicker films. Therefore, the incident angle error, azimuth angle error of polarizer and analyzer, and wavelength error should be firstly calibrated, and the other errors are calibrated.

We have selected the good economic ellipsometric components with the aid of the analysis of errors. Since we especially select the linear sheet polarizer, which has extinction ratio 10E-4, we can save money and make the size of system smaller. At the same way, we can select laser diode in the place of laser. The laser diode is also very cheaper and smaller than laser. Figure 6 shows the error caused by the all errors that we select.

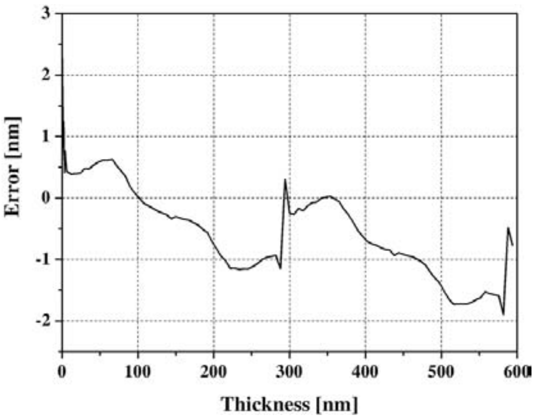


Fig. 6 Simulated thickness error with all errors

4. Optimization Method

There are several errors in ellipsometer, fluctuation of light source, variation of wavelength, extinction ratio and azimuth angle error of polarizer and analyzer, nonlinearity and polarization dependence error of detector, and the random noise errors that are mechanical vibration and fluctuation of environment light, and noise of electric circuit, etc. Residual method can work well when there are only the azimuth angle error and extinction error of polarizer and analyzer, and random noises. When there are variation of wavelength, incident angle error, and the nonlinearity of detector, Residual method could not give the correct azimuth angle of polarizer and analyzer [Fig. 7].

We propose the optimal calibration method that finds least square error between the measured thickness and the simulated thickness. We have modeled the errors of ellipsometric components. We select the error parameters to satisfy the following.

$$\mathit{Minimize}\ \sum_{i=1}^{N}(d^{m}-d^{s})^{2} \tag{10}$$

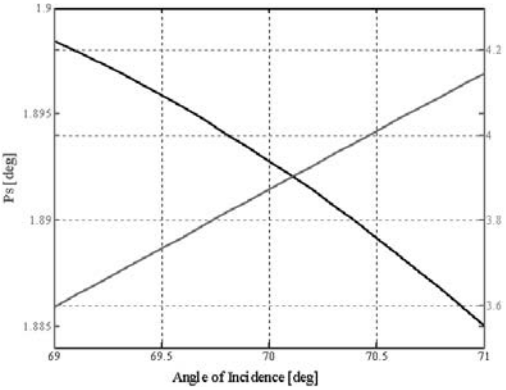


Fig. 7 The calculated reference azimuth angle of polarizer and analyzer by Residual method when there is incident angle error

Table 1 Results of optimization

design variable	unit	initial value	upper bound	lower bound	optimum value
Incident Angle Error	deg	0	2	−2	−0.028
Azimuth Angle Error of Polarizer	deg	0	5	−5	−0.385
Azimuth Error of Analyzer	deg	0	5	−5	2.126

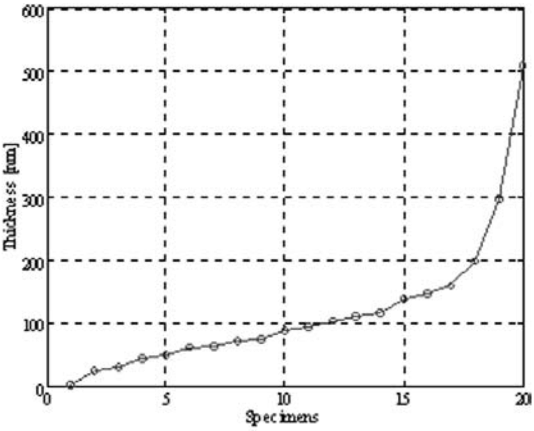


Fig. 8 20 Reference speciments

where N is the nmber of specimen, dm is the measured thickness with CRM and ds is the simulated thickness. We prepared 20 Air-SiO_2Si specimens which were made in Knowledge*On and were measured at KRISS with 0.5 nm standard uncertainty of measurement [Fig. 8], where the conditions of measurement are 70° incident angle, the complex refractive indexes $N_{SiO2}=1.45654$ and $N_{Si}=3.8501-i0.01639$.

The error parameters are too many to run optimal program. From the analysis of errors, we can take some excellent inspirations. First, the polarization of light source does not affect the measurement. The extinction ratios of linear polarizer at analyzer and polarizer very lightly affect the measurement and the extinction ratios are fixedly given so that those can be treated with constant values. The wavelength error of light source is incrementally effective according to the thickness of thin film, and the incident angle error is incrementally and periodically effective according to the thickness of thin film. The azimuth angle errors of polarizer and analyzer are periodically effective according to the thickness of thin film. Therefore, the above stated errors should be optimized firstly. Since the polarization dependence, nonlinearity, bias, and random error of detector are very sensitive on only thin film, the errors of detector have better being optimized later than the previous errors. If wavelength may changes, the complex reflective index changes. Since the wavelength hardly change in practice and the modeling for specimen is not correct, we cannot calibrate the error for wavelength, but put theses to the uncertainty of measurement.

We used Matlab for optimization. Table 1 shows the initial value and upper and lower bound, and optimum value of design variables. The optimum values are slightly different from the results of residual method, and the cost function, standard deviation, is smaller than the result of the residual method. Table 2 shows the

Table 2 Comparisons between each methods

Methods	Standard Uncertainty
A Company	0.3985 nm
No Calibration	0.4599 nm
Residual Calibration	0.2026 nm
Optimal Calibration	0.1894 nm

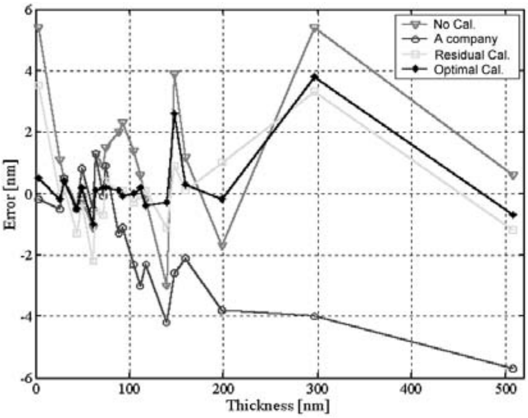


Fig. 9 The calibrated measured thickness errors with respect to CRM

comparisons between each method and between experiment and simulation. Figure 9 show the errors of each method. A careful look at Figure 9 tells that there are some jumps. The reason is also the periodic thickness.

5. Conclusions

We have modeled most errors, which affect measurement, with Jone's matrix. From the simulation, we can characterize the errors and take good aids for selecting components and designing ellipsometer. The traditional residual method has good performance when there are only azimuth angle errors and extinction errors, but it has not good performance when there are other errors. We have proposed the optimal calibration method for overcoming the residual method. The optimal method selects error values to have the least square error between the measured thickness and the simulated thickness. However, the design variables, the errors, are so many that the optimization hardly converges. From the analysis of errors, we have some excellent inspirations. Therefore, we can reduce the design variables to three, incident angle error, and azimuth angle errors of polarizer and analyzer. The optimization results are slightly different from the residual method, and have smaller standard deviation of errors than the residual method. The experiment shows good agreement with the simulations.

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