Analytical solutions of the azimuthal deviation of a polarizer and an analyzer by polarizer–sample–analyzer ellipsometry

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The analytical solutions of the azimuthal deviation of a polarizer and an analyzer were obtained by polarizer–sample–analyzer ellipsometry with a three-intensity measurement technique. By performing two sets of this three-intensity measurement with the polarizer's azimuth set at 45° and at −45°, we were able to obtain a set of ellipsometric parameters free from the azimuthal deviations of the polarizer and the analyzer. © 2006 Optical Society of America

OCIS codes: 120.2130, 120.4290.

1. Introduction

It is known that one can use the ellipsometric parameters Ψ and Δ to deduce optical parameters, such as the complex refractive index and film thickness of a sample.[1] The most important requirement for accurate ellipsometric measurements is calibration of the azimuths of optical components with respect to the plane of incidence. Few calibration techniques have been studied for null[2] and rotating-analyzer ellipsometry,[3] but each of them has to search the position of its minimum intensity to locate the plane of incidence. Instead of using the null technique, Chao *et al.*[4] improved Steel's intensity ratio technique[5] and aligned the azimuths of the polarizer P and of the analyzer A separately to the specimen's surface in a polarizer–sample–analyzer (PSA) system through two incident angles. Moreover, their method can also measure the azimuthal deviation of the polarizer and optimize ellipsometric parameter Ψ by two sets of a three-intensity measurement.[6] Recently we analyzed the effect of the azimuthal deviation of a polarizer to Δ in an imaging ellipsometry[7] and found that this technique is valid as long as the deviation is less than 3°. In theory, these two sets of three-intensity measurements can be used to deduce six parameters simultaneously, but only five of them have been dealt with so far. Now, with the help of the symbolic computer program Mathematica, we have been able to solve the last parameter analytically by means of this three-intensity technique. Instead of using a regression calibration method,[8] we analytically solved Ψ, Δ, and its azimuthal deviations of polarizer α and analyzer β, using the three-intensity measurement technique. Both a numerical simulation and an experimental measurement of the thickness of a SiO_2 thin film on a Si substrate were performed with this technique. Our result is comparable to those measured by other ellipsometers.

2. Theoretical Background

The basic PSA ellipsometer is constructed as shown in Fig. 1(a). Ellipsometric parameters Ψ and Δ are defined as

$$\tan\Psi\exp(i\Delta) = r_p/r_s, \tag{1}$$

where r_p and r_s are the reflection coefficients of the linearly polarized state parallel (p) and perpendicular (s), respectively, to the incident plane. The measured intensity can be written as

$$I(P, A) = I_0(\sin^2 P\sin^2 A + \tan^2\Psi\cos^2 P\cos^2 A + 0.5\tan\Psi\cos\Delta\sin 2P\sin 2A), \tag{2}$$

where azimuths P and A are the transmission axes of the polarizer and the analyzer, respectively. In polar coordinates, if $E_p = E_s$, the reflected intensity is distributed in an elliptical form[6] shown in Fig. 1(b), which can be formulated as

$$I(A) = L\cos^2(A-\theta) + T\sin^2(A-\theta), \tag{3}$$

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Received 13 September 2005; revised 3 January 2006; accepted 7 January 2006; posted 13 January 2006 (Doc. ID 64696).
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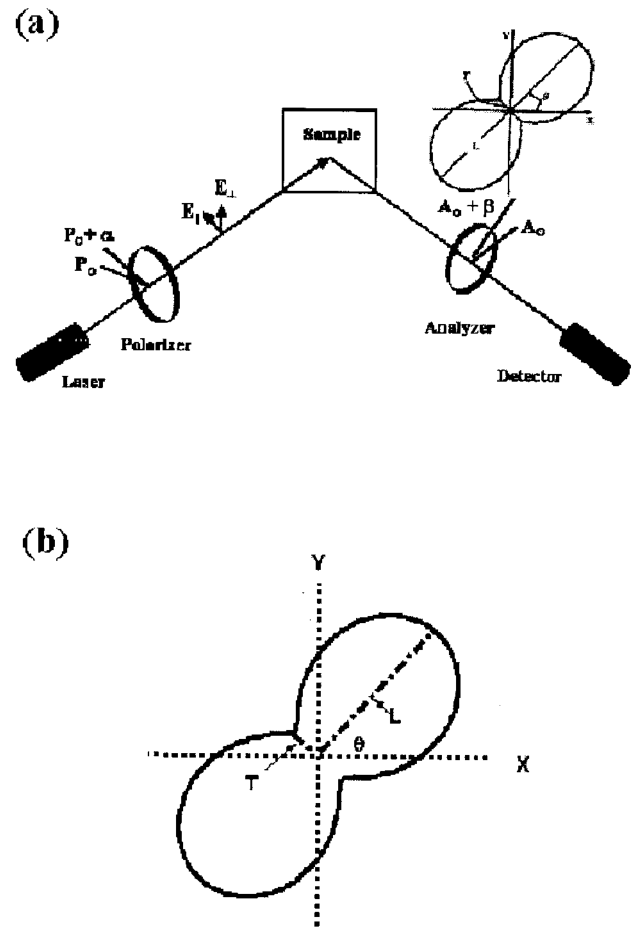

Fig. 1. (a) Schematic setup of the PSA ellipsometer: Laser, He–Ne laser; P, polarizer; A, analyzer; S, sample. (b) Intensity distribution in polar coordinates at various azimuth angles of the analyzer.

where L and T are the magnitudes of the maximum and the minimum intensities, respectively, and θ is the azimuth of maximum intensity. By comparing the coefficients at the same position of A for Eqs. (2) and (3), one can prove that

$$L = I_0\big(\tan^2\Psi\cos^2 P\cos^2\theta + \sin^2 P\sin^2\theta + 0.5\tan\Psi\sin 2P\sin 2\theta\cos\Delta\big), \quad (4)$$

$$T = I_0\big(\tan^2\Psi\cos^2 P\sin^2\theta + \sin^2 P\cos^2\theta - 0.5\tan\Psi\sin 2P\sin 2\theta\cos\Delta\big), \quad (5)$$

$$\tan 2\theta = \frac{\cos\Delta\sin 2P\sin 2\Psi}{\cos 2P - \cos 2\Psi}. \quad (6)$$

Performing complicated trigonometric manipulations from Eq. (4) to (6), one can prove that

$$\frac{(L-T)^2}{4LT}\sin^2(2\theta) = \cot^2\Delta. \quad (7)$$

Moreover, Eq. (3) is further simplified as

$$I(A) = B(1 + C\cos 2A + D\sin 2A), \quad (8)$$

where the parameters B, C, and D can be written in terms of L, T, and θ, i.e., $B = 0.5(L + T)$, $C = (L - T)\cos 2\theta/(L + T)$, and $D = (L - T)\sin 2\theta/(L + T)$. From Eq. (8) it is easy to prove that parameters B, C, and D can be measured by use of three intensities measured at $A = 0°, 60°, 120°$:

$$B = \frac{1}{3}[I(0) + I(60) + I(120)],$$

$$C = 2 - \frac{1}{B}[I(60) + I(120)],$$

$$D = \frac{1}{B\sqrt{3}}[I(60) - I(120)],$$

and the following:

$$\tan 2\theta = \frac{D}{C}, \quad L = \frac{DB}{\sin 2\theta} + B, \quad T = 2B - L. \quad (9)$$

Rewriting Eq. (2) in terms of $\cos 2A$ and $\sin 2A$ and comparing the result with Eq. (8), one can also prove that

$$\tan^2\Psi = \frac{1+C}{1-C}\tan^2 P. \quad (10)$$

If P and A are well aligned to the plane of incidence, one can obtain B, C, and D by making three intensity measurements and then derive the values of θ, L, and T from Eqs. (9); using Eqs. (6) and (10), one can deduce the ellipsometric parameters from the parameters obtained. It is known that precise alignment is almost impossible to achieve; just as for the zone average in null ellipsometry, we assume that the deviation of the polarizer is α and then expand analytic equation (10) as follows:

$$P = 45° + \alpha, \qquad \tan^2\Psi = \left(\frac{1+C}{1-C}\right)\frac{1+\sin 2\alpha}{1-\sin 2\alpha},$$

$$P = -45° + \alpha, \qquad \tan^2\Psi = \left(\frac{1+C'}{1-C'}\right)\frac{1-\sin 2\alpha}{1+\sin 2\alpha}, \quad (11)$$

where C and C' are the corresponding parameters at $P = 45°$ and $P = -45°$, respectively. Instead of using a regression technique,[8] one can eliminate the systematic error in Ψ by taking the product of these two sets of three-intensity measurements[6]: We also can obtain its deviation α by taking the ratio of the same measurements. For solving the azimuth deviation of analyzer β, one also can modify Eq. (7) as

$$\frac{(L - T)^2}{4LT} \sin^2 2(\theta + \beta) = \cot^2 \Delta. \qquad (12)$$

According to Eq. (6), one can prove that $\tan 2\theta_1 = -\tan 2\theta_2$, where θ_1 and θ_2 are the azimuths between the incident plane and the maximum intensity when the azimuth of the polarizer is set at 45° and −45°, respectively. By substituting the corresponding parameters L_1, T_1 and L_2, T_2 into Eq. (12), one can prove that

$$\tan 2\beta = -\frac{(L_2 - T_2)\sin 2(\theta_2)/2\sqrt{L_2T_2} + (L_1 - T_1)\sin 2(\theta_1)/2\sqrt{L_1T_1}}{(L_1 - T_1)\cos 2(\theta_1)/2\sqrt{L_1T_1} + (L_2 - T_2)\cos 2(\theta_2)/2\sqrt{L_2T_2}}. \qquad (13)$$

One can correct the measured θ by subtracting deviation β obtained from Eq. (13). The value of C can be further corrected from the correction of θ; i.e., $C_{corr} = C \cos 2(\theta - \beta)/\cos 2\theta$; then one can obtain a fully corrected value of Ψ. Because one can have exact values of P (from the correction of α), θ, and Ψ, one can deduce the value of Δ from Eq. (6) and be free from the azimuthal errors of polarizer and analyzer. To understand the effect of this analytical method, we simulated an intensity distribution from Eq. (2) by assuming that $\Psi_{th} = 30°$ and $\Delta_{th} = 140°$. The intensity values were obtained from the distribution at $P = \pm 45° + \alpha$ (where α varies from −5° to 5°) and $A = 0° + \beta$, $60° + \beta$, and $120° + \beta$ (where β varies from −5° to 5°). The accuracy of Ψ and Δ was analyzed by two optimization methods[7] through numerical simulation. In the beginning, we analyzed the system errors of Ψ and Δ by eliminating α in Eqs. (11) to improve the value of Ψ and using $\theta_{ave} = (180 - \theta_2 + \theta_1)/2$ in Eq. (6) to calculate the value of Δ; we then compared Ψ and Δ with Ψ_{th} and Δ_{th}, respectively, by plotting $\delta\Psi(\Psi_{th} - \Psi)$ and $\delta\Delta(\Delta_{th} - \Delta)$ for β = 0 for various values of α [Fig. 2(a)] and for α = 0 for various values of β [Fig. 2(b)]. We also graphed these system errors in a two-dimensional distribution of α and β, as shown in Figs. 2(c) and 2(d). Figure 2 clearly demonstrates the system errors caused by misalignment of α and β, which provided the motivation for this analytical method to be developed. Finally, we analyzed the system errors by determining the value of β from Eq. (13) and the value of α from Eqs. (11) to obtain the analytical values of θ, Ψ, and Δ; these analytically solved ellipsometric parameters are compared in Fig. 3 with their theoretical values.

3. Experiment

We used a marked polarizer (Melles Griot sheet polarizer) to locate the minimum reflection at the Brewster angle of a nonabsorbent material, which we considered the reference zero. The azimuth angles of the polarizer and the analyzer were located by their minimum transmission by use of a powermeter (Thorlabs PDA55) and then were digitized by a multimeter (Keithley 195A). After the rough alignment, the light beam (Melles Griot 05-STP-901, λ = 632.8 nm stabilized He–Ne laser) was set at the incident angle of 70° (69.94° was used as the incident angle for the thickness deduction; according to Ref. 9, rotation of the polarizer can cause the beam to deviate from 70°) and passed through a polarizer with its azimuth set at ±45°. The analyzer was mounted on a motor-

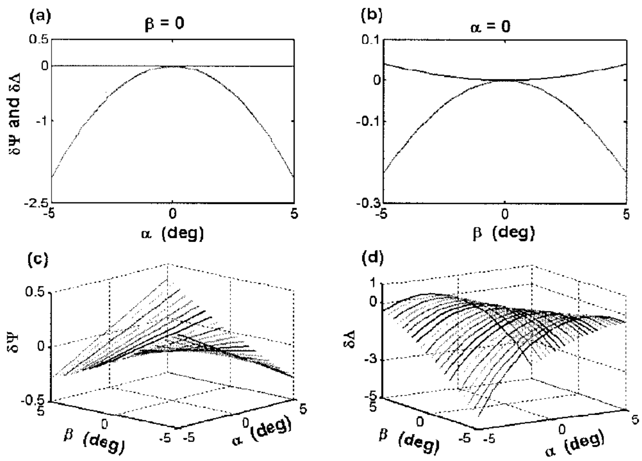

Fig. 2. Numerical simulation for analyzing the systematic errors of Ψ and Δ by eliminating α to improve the value of Ψ and using $\theta_{ave} = (180 - \theta_2 + \theta_1)/2$ to calculate Δ through the three-intensity measurement technique: (a) δΨ and δΔ versus α as β = 0, (b) δΨ and δΔ versus β as α = 0, (c) δΨ versus α and β, (d) δΔ versus α and β. The theoretical values of Ψ_{th} and Δ_{th} are 30° and 140°, respectively.

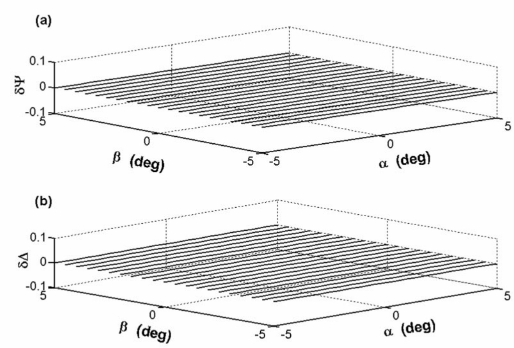

Fig. 3. Numerical simulation for analyzing the systematic errors of Ψ and Δ by this analytical method: (a) δΨ versus α and β; (b) δΔ versus α and β.

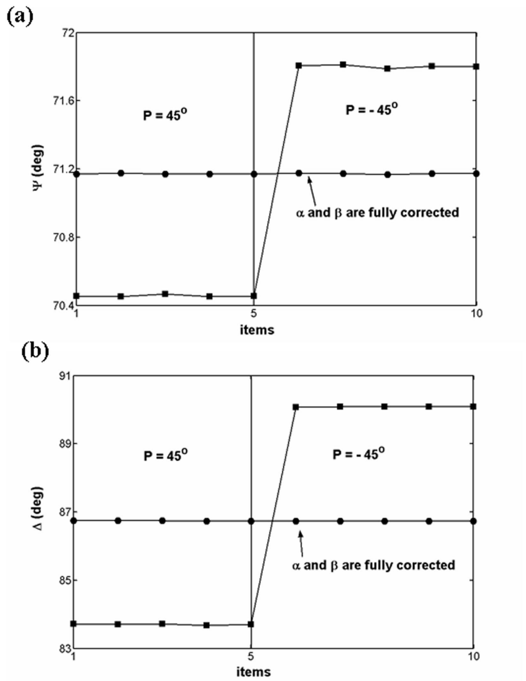

Fig. 4. Ellipsometric measurements of PSA ellipsometry for a SiO_2 film on a Si substrate: (a) Ψ and (b) Δ measured after a rough alignment (filled squares) at $P = 45°$ and at $P = -45°$, where $\alpha = 0.998 \pm 0.011°$ and $\beta = -1.233 \pm 0.005°$ and after readjusted alignment (filled circles) at $P = 45°$ and at $P = -45°$, where $\alpha = 0.015 \pm 0.009°$ and $\beta = -0.006 \pm 0.003°$.

controlled rotator, and three radiances were obtained with the azimuths of the analyzer set at 0°, 60°, and 120°. All intensities were measured and stored in a PC for calculating the values of β, α, Ψ, and Δ. For comparison, we measured a standard SiO_2 thin film on a Si substrate whose thickness measured by this technique was compared with that measured by a commercial ellipsometer (Jobin-Yvon spectroscopic phase-modulated ellipsometer). To prove the validity of this analytic technique, we repeated the measurement after readjusting the azimuth angle of the polarizer and analyzer to zero, in accordance with previous experimental results.

4. Results and Conclusions

Our primary objective was to compare the ellipsometric parameters measured with rough alignment with the analytically corrected values. Just as expected, the system errors were clearly observable in the deduced values of Ψ and Δ, measured at $P = 45°$ and $P = -45°$ separately, as shown in Fig. 4, and their differences vanished after we readjusted the zero of P back by 1° and of A forward by 1.23°. However, the corrected ellipsometric parameters of the results deviated from each other by less than 0.01°, as shown in Tables 1 and 2. Instead of using a regression calibration method, we can analytically solve Ψ, Δ, and the azimuthal deviations of the polarizer and analyzer, by using two sets of the three-intensity measurement technique, which not only reduces the number of measurements needed for calculating the ellipsometric parameters without losing accuracy but also directly determines the azimuthal deviations of polarizer and analyzer relative to the plane of incidence; i.e., the reference zero. Since the PSA configuration is the backbone of the technology of ellipsometry, once the reference zero is obtained, the optic axis of the compensator–phase modulator[10] can be aligned accordingly. Because only six intensity measurements are needed to deduce the ellipsometric parameters accurately, one can easily convert this three-intensity

Table 1. Optimized Ellipsometric Measurements of PSA Ellipsometry for a SiO_2 Film on a Si Substrate after Rough Alignment

Experiment	Ψ (deg)	Δ (deg)	Thickness (nm)	α (deg)	β (deg)
1	71.172	86.742	129.89	0.993	−1.229
2	71.175	86.745	129.93	1.000	−1.234
3	71.169	86.754	129.85	0.968	−1.231
4	71.171	86.727	129.88	0.991	−1.241
Mean	71.171	86.741	129.88	0.988	−1.233
Standard deviation	0.003	0.011	0.03	0.011	0.005
Jobin-Yvon ellipsometer			129.3		

Table 2. Optimized Ellipsometric Measurements of PSA Ellipsometry for a SiO_2 Film on a Si Substrate after Readjusting Azimuth Angles of Polarizer and Analyzer According to the Measured Value, i.e., the Zero of *P* Backed Up by 1° and of *A* Forwarded by 1.23°

Experiment	Ψ (deg)	Δ (deg)	Thickness (nm)	α (deg)	β (deg)
1	71.176	86.739	129.94	0.017	−0.011
2	71.174	86.731	129.93	0.013	−0.005
3	71.166	86.728	129.87	0.003	−0.005
4	71.174	86.726	129.91	0.026	−0.004
Mean	71.173	86.731	129.91	0.015	−0.006
Standard deviation	0.004	0.006	0.03	0.009	0.003
Jobin-Yvon ellipsometer			129.3		

measurement technique to be an imaging ellipsometry.[7] We already have proved that the azimuthal deviation of a polarizer is related to the normal direction of the incident plane, so one can employ the imaging ellipsometry to measure the refractive index profile of a curved surface[11] to further study thin-film coating on a lens.

The most important aspect of this technique is the concept of direct determination, in contrast to locating the minimum intensity in null ellipsometry, which not only requires a sensitivity detector but also requires that the polarizer have a high extinction ratio. The technique proposed here needs a minimum amount of data to deduce the deviations and ellipsometric parameters simultaneously and with high accuracy, but it does require a high dynamic range to achieve high precision. Moreover, a complicated alignment process is not needed in the simple PSA ellipsometry.

This research is supported by the National Science Council of the Republic of China by grant NSC93-2215-E009-056.

References

1. R. M. A. Azzam and N. M. Bashara, *Ellipsometry and Polarized Light* (North-Holland, 1980), p. 387.
2. F. L. McCrackin, "Analyses and corrections of instrumental errors in ellipsometry," J. Opt. Soc. Am. **60,** 57–63 (1970).
3. B. J. Stagg and T. T. Charalampopoulos, "Method for azimuthal alignment in fixed-angle ellipsometry," Appl. Opt. **4,** 479–484 (1992).
4. Y. F. Chao, C. S. Wei, W. C. Lee, S. C. Lin, and T. S. Chao, "Ellipsometric measurements and its alignment-Using the intensity ratio technique," Jpn. J. Appl. Phys. **34,** 5016–5019 (1995).
5. M. R. Steel, "Method for azimuth alignment in ellipsometry," Appl. Opt. **10,** 2370–2371 (1971).
6. Y. F. Chao, W. C. Lee, C. S. Hung, and J. J. Lin, "A three-intensity technique for polarizer–sample–analyser photometric ellipsometry and polarimetry," J. Phys. D Appl. Phys. **31,** 1968–1974 (1998).
7. Y. F. Chao and K. Y. Lee, "Index profile of radial gradient index lens measured by imaging ellipsometric technique," Jpn. J. Appl. Phys. **44,** 1111–1114 (2005).
8. B. Johs, "Regression calibration method for rotating element ellipsometers," Thin Solid Films **234,** 395–398 (1993).
9. Y. F. Chao, M. W. Wang, and Z. C. Ko, "An error evaluation technique for the angle of incidence in a rotating element ellipsometer using a quartz crystal," J. Phys. D Appl. Phys. **32,** 2246–2249 (1999).
10. M. W. Wang and Y. F. Chao, "Azimuth alignment in photoelastic modulation ellipsometry at a fixed incident angle," Jpn. J. Appl. Phys. **41,** 3981–3986 (2002).
11. K. Y. Lee and Y. F. Chao, "The ellipsometric measurements of a curved surface," Jpn. J. Appl. Phys. **44,** L1015–L1018 (2005).