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Measurement of ellipsometric data and surface orientations by modulated circular polarized light

Messung von ellipsometrischen Daten und Oberflächenorientierungen durch moduliertes zirkular polarisiertes Licht

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Abstract: Ellipsometry is a widely used optical method for the characterization of materials and thin films. However, only flat or nearly flat surfaces can be measured since small deviations of the angle of incidence might lead to significant experimental errors. In order to overcome the geometrical limitations of ellipsometry, the retroreflex ellipsometry developed at Fraunhofer IOSB is used. Based on this configuration, a new illumination method is proposed. When the sample is illuminated by modulated circular polarized light (LCP and RCP), the ellipsometric parameters (Ψ , Δ) and the tilted angle (Φ) can be determined directly. Combined with reflectance measurement or prior knowledge of optical properties of samples, the surface orientation can be obtained.

Keywords: Retroreflex ellipsometry, modulated circular polarized light, curved surfaces.

Zusammenfassung: Ellipsometrie ist ein weit verbreitetes optisches Verfahren zur Charakterisierung von Materialien und Beschichtungen. Es können jedoch nur flache oder nahezu flache Oberflächen gemessen werden, da bereits eine geringe Abweichung des Einfallswinkels zu signifikanten Messabweichungen führen kann. Um die geometrischen Grenzen der Ellipsometrie zu überwinden, wird die am Fraunhofer-IOSB entwickelte Retroreflexellipsometrie eingesetzt. Basierend auf dieser Konfiguration wird ein neues Beleuchtungsverfahren vorgeschlagen. Wenn die Probe mit moduliertem zirkular polarisiertem Licht (LCP und RCP)

beleuchtet wird, können die ellipsometrischen Parameter (Ψ , Δ) und der Neigungswinkel (Φ) direkt bestimmt werden. In Kombination mit Remissionsmessungen oder bei Kenntnis der optischen Eigenschaften von Proben, kann deren Oberflächenorientierung ermittelt werden.

Schlüsselwörter: Retroreflex-Ellipsometrie, moduliertes zirkular polarisiertes Licht, gekrümmte Oberflächen.

1 Introduction

Ellipsometry is a widely used optical method for characterizing materials and thin films. The advantages of ellipsometry are high precision and non-destructive measurements [1] that might be used for process monitoring [2]. Ellipsometers can be used in various application fields, e.g., semiconductor, chemical, and display industry. Ellipsometers measure the polarization change due to the reflection or transmission at samples. The reflected or transmitted light from a sample is usually classified as p- and s-polarized light (parallel or perpendicular to the plane of incidence). In a reflection setup, the ellipsometric parameters (Ψ , Δ) are defined as [1]

$$\rho = \frac{r_p}{r_s} = \tan \Psi e^{i\Delta}, \quad (1)$$

where r_p and r_s are amplitude reflection coefficients for p- and s-polarized light. Ψ and Δ represent the amplitude ratio and the phase difference. If the sample is an isotropic substrate, the complex refractive index $\bar{n}_t$ can be expressed by ellipsometric parameters (Ψ , Δ) and the angle of incidence θ as [1]

$$\bar{n}_t = \bar{n}_i \tan \theta \sqrt{1 - \frac{4\rho}{(1 + \rho)^2} \sin^2 \theta}, \quad (2)$$

where $\bar{n}_i$ is the refractive index of ambient (usually air). The refractive index of air is $n = 1.0003$ [3] which is almost the same value as $n = 1$ in vacuum.

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However, conventional ellipsometers can measure only flat or nearly flat surfaces because the measurement configuration is based on the reflection principle. A small deviation of the angle of incidence might lead to significant experimental errors. The acceptable tolerance of the angle deviation is usually less than 1° . If the angle deviation is over the acceptable range, the detector cannot receive any signal. There have been several studies using ellipsometry to measure non-planar surfaces [4–7]. They measured the azimuthal deviations of the optical elements in their systems because the deviations are related to the surface geometry. Nevertheless, there are some constraints in these studies, e.g., small measurement ranges of angle deviations of the surface, special requirements for the illumination, complicated system design, or prior knowledge of refractive indices of samples. In order to overcome these restrictions, retroreflex ellipsometry was developed at Fraunhofer IOSB [8, 9]. In this configuration, a retroreflective film, which contains micron glass beads, is used to reflect the light from the sample back to the detector on the same path. The polarization effect of the retroreflective film is the same as that of an ideal mirror [10]. The acceptable angle deviation of the surface is up to 30° , which provides a large measurement range of angle deviations of the surface and simplifies the alignment procedure between the sample and the detector. Based on this configuration, we propose a new method to measure optical properties and surface orientations for isotropic materials by modulated circular polarized light.

2 Principle of retroreflex ellipsometry

Figure 1 shows the schematic of the retroreflex ellipsometry. The setup is a return-path configuration in which a retroreflective film reflects the light from the sample back to the transceiver on the same beam path respectively.

Fig. 1: The schematic of retroreflex ellipsometry, where $\vec{E}_{ill}$ and $\vec{E}_{det}$ are Stokes vectors of illumination and detected beams.

After the retroreflection, the light beam only has a phase difference of 180° (i.e., an effect as an ideal mirror). The transceiver includes a two-state polarization state generator (modulator), a polarization state analyzer and a non-polarizing beamsplitter (NPBS). The generator can generate left circular polarized (LCP) light and right circular polarized (RCP) light. The analyzer can measure the stoke vector of the reflected light from the sample. The construction of this system is simple because the illumination and the detector are integrated in one unit. Another advantage of this device is the higher sensitivity to the optical properties of surfaces than conventional ellipsometers because the polarization effects of the sample occur on the path to the retroreflective film and the path back to the transceiver.

As shown in Figure 2, if a flat sample defines the xy -plane, the z -axis is the surface normal. While the sample rotates about the y -axis, the surface normal of the sample becomes the vector $\vec{n}$. We can define the tilted angle ϕ as the included angle between the surface normal $\vec{n}$ and the z -axis, and the angle of incidence θ as the included angle between the surface normal $\vec{n}$ and the incident beam.

The polarization effect of optical elements or interaction at boundaries can be described by Stokes vectors and Mueller matrices. Stoke vectors describe the polarization state of light beams. Mueller matrices describe the characteristics of the altering of Stokes vectors at or in a material. The Mueller matrix of an isotropic sample can be expressed as

$$\mathbf{M}_s = \begin{bmatrix} 1 & -N & 0 & 0 \\ -N & 1 & 0 & 0 \\ 0 & 0 & C & S \\ 0 & 0 & -S & C \end{bmatrix}, \quad (3)$$

where $N = \cos 2\Psi$, $S = \sin 2\Psi \sin \Delta$, and $C = \sin 2\Psi \cos \Delta$. The Mueller matrix of azimuthal rotation can be described as

$$\mathbf{M}_R(\alpha) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\alpha & -\sin 2\alpha & 0 \\ 0 & \sin 2\alpha & \cos 2\alpha & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad (4)$$

The polarization model of the measurement in Figures 1 and 2 can be described by the Mueller formalism [11]:

$$\mathbf{M} = \mathbf{M}_R(det) \cdot \mathbf{M}_S \cdot \mathbf{M}_{RR} \cdot \mathbf{M}_S \cdot \mathbf{M}_R(ill). \quad (5)$$

$\mathbf{M}_{RR}$, $\mathbf{M}_R(ill)$, and $\mathbf{M}_R(det)$ are the Muller matrices of the retroreflective film and the azimuthal rotation matrices of the illumination and the detector. $\mathbf{M}_{RR}$ is a diagonal matrix, where the diagonal elements are 1, 1, -1 , and

$$\mathbf{M} = \begin{bmatrix} 1 + N^2 & -2N \cos 2\phi & 2N \sin 2\phi & 0 \\ -2N \cos 2\phi & (1 - S^2) + (1 - C^2) \cos 4\phi & -(1 - C^2) \sin 4\phi & 2CS \sin 2\phi \\ -2N \sin 2\phi & (1 - C^2) \sin 4\phi & -(1 - S^2) + (1 - C^2) \cos 4\phi & -2CS \cos 2\phi \\ 0 & 2CS \sin 2\phi & 2CS \cos 2\phi & S^2 - C^2 \end{bmatrix} \quad (6)$$

Fig. 2: Schematic of the flat sample rotates about the y-axis.

–1. If the system is well aligned, $\mathbf{M}_R(ill) = \mathbf{M}_R(det) = \mathbf{M}_R(\phi)$. If the measurement has no depolarization, $N^2 + S^2 + C^2 = 1$. Then the matrix $\mathbf{M}$ can be simplified as shown in Eq. 6. Structural anisotropy can be observed because the surface normal is tilted. The two polarization states of the illumination used in this paper are LCP and RCP light which are defined as: $\mathbf{LCP} = [1 \ 0 \ 0 \ 1]^T$ and $\mathbf{RCP} = [1 \ 0 \ 0 \ -1]^T$. The measurement result at LCP and RCP illumination are denoted as $\vec{E}_{LCP}$ and $\vec{E}_{RCP}$. The difference of $\vec{E}_{LCP}$ and $\vec{E}_{RCP}$ can be expressed as

$$\vec{E}^- = \vec{E}_{LCP} - \vec{E}_{RCP} = \begin{bmatrix} 0 \\ \frac{4 \sin 2\phi \sin^2 2\Psi \sin 2\Delta}{3 + \cos 4\Psi} \\ \frac{4 \cos 2\phi \sin^2 2\Psi \sin 2\Delta}{3 + \cos 4\Psi} \\ \frac{4 \cos 2\Delta \sin^2 2\Psi}{3 + \cos 4\Psi} \end{bmatrix}. \quad (7)$$

The ratios between $\vec{E}^-(2)$ and $\vec{E}^-(3)$, and $\vec{E}^-(3)$ and $\vec{E}^-(4)$ are expressed as

$$\frac{\vec{E}^-(2)}{\vec{E}^-(3)} = \tan 2\phi \quad (8)$$

$$\frac{\vec{E}^-(3)}{\vec{E}^-(4)} = \cos 2\phi \tan 2\Delta \quad (9)$$

At modulated circular polarized light, ϕ , Ψ , and Δ can be solved by Eqs. 7, 8 and 9. For samples with known refractive index, the angle of incidence θ can be directly obtained by Fresnel's equations [5]. For samples with unknown refractive index, the knowledge of θ is essential. In order to obtain θ for unknown refractive indices, measurements of reflectance R can be used. R , Ψ , and Δ are functions of the complex refractive index $\bar{n}$ and the angle

of incidence θ . Thus, $\bar{n}$ and θ can be solved simultaneously. The modulated circular polarized illumination provides a simple acquisition method for determining ellipsometry data (Ψ, Δ), surface orientation (ϕ, θ), and the complex refractive index $\bar{n}$ of surfaces in parallel.

3 Simulation results

Figure 3 shows a specular surface reflection at a metallic sphere with modulated circular polarized illumination. The sphere lies on the xy-plane and the transceiver moves along the x- and the y-axes. Figure 4(a) shows the simulation result of the scanning along the x-axis ($y = 0$). During the x-axis scanning, only the angles of incidence change while the tilt angle keeps the same ($\phi = 0$). Therefore, $\vec{E}^-(2)$ is zero. Figure 4(b) demonstrates the simulation result of the scanning along the y-axis ($x = 0$). The changes of the tilted angles can be observed by $\vec{E}^-(2)$. In the y-axis scanning, the tilted angle ϕ changes from -10° to 10° and the angles of incidence have slight altering ($< 0.35^\circ$). Thus, $\vec{E}^-(4)$ has only 0.04 difference during the scanning.

Fig. 3: A specular surface reflection at a metallic sphere with modulated circular polarization illumination. The refractive index of the metallic surface is 0.18377-3.4313i. The angle of incidence and the tilted angle at (0,0,50) are 70° and 0° .

Fig. 4: (a) The simulation result of the scanning along x axis ($y=0$). (b) The simulation result of the scanning along y axis ($x=0$).

4 Experiment results

To evaluate the proposed method, an unprotected gold mirror (PF10-03-M03, Thorlabs, Inc.) was tested. First, the mirror was measured by a commercial ellipsometer (Smart SE, HORIBA Scientific) to get the complex refractive index. The measurement result of the unprotected gold mirror is $0.13204 - 3.07747i$ at a wavelength of 637.1 nm. The mirror changes the angle of incidence from 65° to 70° at a tilted angle of 0° and is measured by the retroreflex ellipsometer with modulated circular polarized light at a wavelength of 637.1 nm. Finally, the result was compared with theoretical values which are calculated by Fresnel's equations. Figure 5 shows the measurement result of the unprotected gold mirror. The tilted angles should keep the same during the change of the incident angle. Since the tilted angle ϕ is 0° , $\vec{E}^-(2)$ should be 0. The measurement result shows a good correspondence to the theory. While the angle of incidence increased, the phase difference Δ decreased. Thus, $\vec{E}^-(3)$ increased and $\vec{E}^-(4)$ decreased. The measurement result corresponds to the simulation results which are calculated in the previous section. Table 1 lists the calculation results of Ψ , Δ and Φ . Figure 6 shows the comparison between theoretical and measured values. The mean absolute errors of amplitude ratio Ψ and phase difference Δ are 0.29° and 0.35° .

The observed deviations are not too large for many applications. Nevertheless, they indicate systematic errors that should be eliminated. The most probable error source in the actual setup of the retroreflex ellipsometer is the NPBS. The function of the NPBS is to transmit the beam

of the source to the sample and reflect the beam from the sample to the detector. Johs and He [11] mentioned that a NPBS induces polarization distortion. Liu et al. [12] measured the Mueller matrices of a NPBS in transmission and reflection for compensating the polarization distortion. Therefore, the polarization effect of the NPBS cannot be neglected.

Fig. 5: The difference of $\vec{E}_{LCP}$ and $\vec{E}_{RCP}$ of the unprotected gold mirror at modulated circular polarized light.

Fig. 6: The experimental result of the unprotected gold mirror and the theoretical values calculated by Fresnel's equations.

Table 1: Calculation result of Ψ , Δ and Φ .

AOI (deg)	Ψ (deg)	Δ (deg)	ϕ (deg)
66	43.97	114.85	-0.43
67	43.95	111.98	-0.42
68	43.93	108.97	-0.47
69	43.91	105.82	-0.49
70	43.90	102.53	-0.62

5 Conclusions

The principle of the retroreflex ellipsometry allows ellipsometry to be used in real industrial applications, e.g., inline workpiece inspection for planar or nonplanar surfaces, process control in roll-to-roll manufacturing processes, and film thicknesses measurements on automobile parts. The measurement results in this paper prove that using the retroreflex ellipsometer with modulated circular polarized light can directly measure ellipsometric parameters (Ψ , Δ) and the tilted angle ϕ for isotropic materials. Combined with the reflectance measurement or prior knowledge of material properties, the surface orientation and the complex refractive index can be obtained. Moreover, the proposed method reduces the measurement time because only two Stokes vectors are necessary for the calculation. The measurement results of an unprotected gold mirror yields small errors in the amplitude ratio Ψ and the phase difference Δ . In future investigations, we plan to characterize and compensate the polarization distortion of the NPBS to improve the performance of the retroreflex ellipsometer, and apply the proposed method to thin-film systems.

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