The ellipsometric measurements on SiO2 by intensity ratio technique

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ABSTRACT

A PSA photometric ellipsometric technique is used to measure the ellipsometric parameters, ψ and Δ. Taking intensity ratios of $A = \frac{I(\pi/4+dp,dA)}{I(\pi/4+dp,\pi/2+dA)}$ and $B = \frac{I(-\pi/4+dp,dA)}{I(-\pi/4+dp,\pi/2+dA)}$ to their first order approximation under small azimuth deviations of polarizer (dp) and analyzer (dA), we find that at fixed dA these two ratios have opposite gradient with respect to dp and intersect to each other at a special dp where $A = B = \tan^2 \psi$, and the position of this dp is linearly related to $\cos \Delta$. For comparison, $\psi$ and $\Delta$ of a SiO2/Si thin film are measured by conventional null ellipsometry and intensity ratio technique. An higher percentage error on $\Delta$ is expected for this PSA system. The source of errors will be discussed.

Keyword: Ellipsometry, thin film

INTRODUCTION

It is known that ellipsometric parameters $\psi$ and $\Delta$ can be used to deduce the optical constants (e.g., complex refractive index, film thickness) of the sample. The basic requirement in ellipsometric measurement is to calibrate the azimuths of optical components with respect to the surface of specimen, which has been widely studied both in null and rotating-analyzer ellipsometry (RAE). The accuracy of azimuths of polarizer and analyzer has hardly ever been discussed in the static photometric ellipsometry, which is used more often for remote sensing as polarimeter, where the spatial polarization difference is the primary interest rather than the polarization changes through a medium. It is our interest to convert this type of polarimeter into a static photometric ellipsometer so that it can be used for the study of static samples in the laboratory. Steel aligned the transmission axis of analyzer and polarizer with respect to the reflecting surface by an intensity ratio technique under the assumption that azimuths of polarizer and analyzer can be well aligned by a straight-through method. Using the apparatus available to us, we can only align the azimuth angle of polarizer to that of analyzer within 1° of accuracy. Since the azimuths of polarizer and analyzer are independent to each other, we separately consider the azimuth-angle errors of polarizer and analyzer with respect to the reflecting surface. Using the intensity ratio technique, we can systematically align the system within 0.02°.

In the process of alignment, one have to find the intersection of two intensity ratios which not only can be used to locate the transmission axes of polarizer and analyzer with respect to the reflection surface of the sample, it also reveal the value of $\tan^2 \psi$. We shall prove this can be obtained when azimuth-angles of polarizer and analyzer within 1° of accuracy, e.g., the intensity ratio linearly varies with respect to the deviation of their azimuth angles.
The ellipsometric parameters $\psi$ and $\Delta$ are defined as $\tan \psi e^{i\Delta} = r_p / r_s$, where $r_p$ and $r_s$ are the reflection coefficients in the planes parallel (p) and perpendicular (s) to the plane of incidence, respectively. The Müller matrix of an isotropic medium is

$$
\begin{bmatrix}
1 & -\cos 2\psi & 0 & 0 \\
-\cos 2\psi & 1 & 0 & 0 \\
0 & 0 & \sin 2\psi \cos \Delta & \sin 2\psi \sin \Delta \\
0 & 0 & -\sin 2\psi \sin \Delta & \sin 2\psi \cos \Delta
\end{bmatrix}
$$

The Stokes vector of a polarizer is

$$\tilde{S}(p) = \left[ 1 \ \cos 2p \ \sin 2p \ 0 \right] ,$$

where $p$ is the azimuth angle and $\varphi$ is the degree of polarization of the polarizer. If we take $\varphi = 1 - \delta \xi$, one can prove that the intensity measured from a PSA (polarizer-sample-analyzer) system is

$$I(P,A) = \frac{I_0}{\cos \Delta \sin 2P \sin 2 \Delta } \{ \sin^2 P \sin^2 A + \tan^2 \psi \cos^2 P \cos^2 \Delta + 0.5 \tan \psi \cos \Delta \sin 2P \sin 2 \Delta \} + O(\delta \xi)$$

where $P$ and $A$ are azimuths of polarizer and analyzer, respectively. The polarizer and analyzer can be coarsely aligned to the reflecting surface by using the Brewster angle of a testing plate. Let $\alpha$ and $\beta$ be the small angle deviations from the reflecting surface for the polarizer and analyzer, respectively. The intensity ratios are defined as

$$A(\alpha, \beta) = I_2(\pi/4 + \alpha, \beta) / I_1(\pi/4 + \alpha, \pi/2 + \beta) ,$$
$$B(\alpha, \beta) = I_2(-\pi/4 + \alpha, \beta) / I_1(-\pi/4 + \alpha, \pi/2 + \beta) .$$

These intensity ratios can be expanded to the first order approximation around their respective scales, that is around $I_2(\pi/4, 0) / I_1(\pi/4, \pi/2)$ and $I_2(-\pi/4, 0) / I_1(-\pi/4, \pi/2)$, one can have the following expressions in their first order approximation,

$$A(\alpha, \beta) \sim \frac{\tan^2 \psi - 2 \tan^2 \psi \alpha - \sec^2 \psi \tan \psi \cos \Delta \beta}{2 \tan^2 \psi \alpha - \sec^2 \psi \tan \psi \cos \Delta \beta} .$$

These two linear equations have opposite gradient and intersect with each other at

$$[ 2 \tan^2 \psi \alpha - \sec^2 \psi \tan \psi \cos \Delta \beta ] = 0 .$$
and thus have the same value of $\tan^2 \psi$. The linear relation of eq.(5) is proportion to $\cos \Delta$ of the medium. The slope of eq.(5) $d\alpha/d\beta$ presents opposite sign as the incident light across the principle angle $\theta_p$. This phenomenon is clearly observable for nonabsorbing materials across the Brewster angle, which coincides with its principle angle. The solution of eq. (5) for incident angles $\theta_i$ greater and less than $\theta_p$, the intersection of these two lines will reveal the incident plane of the measuring sample.

**NUMERICAL SIMULATION**

Only bulk media are considered (Fig. 1). (a) A thick glass plate of refractive index 1.5 is taken for nonabsorbing material. The exact and first order approximation of intensity ratios A and B can be calculated by considering $\cos \Delta = -1$ for $\theta_i < \theta_p$ and $\cos \Delta = 1$ for $\theta_i > \theta_p$. The linear property of A and B is valid only in the vicinity of its intersection such as in Fig. 2. (b) An air/gold interface of refractive index 0.35 - i 2.45 is considered to be the absorbing material. For $\theta_i < \theta_p$, we take $\theta_i = 45^\circ$ for both cases. Because of avoiding the principle angle, where $\cos \Delta$ will approach to zero, we take $\theta_i = 70^\circ$ for glass and $\theta_i = 75^\circ$ for air/gold interface for $\theta_i > \theta_p$. At fixed $\beta$, the incident plane is in between the intersections of intensity ratios A and B for $\theta_i < \theta_p$ and $\theta_i > \theta_p$, these intersections will switch side with respect to the incident plane when $\beta$ changes sign, shown as Fig. 3a-3b. This processes not only provide the direction of $\beta$, the separation of intersections will also give the information of how close the laboratory scale to the incident plane.

**EXPERIMENTAL SETUP**

Fig. 1 shows the experimental setup. A He-Ne laser is used as the light source for the PSA system. Intensities of $I (\pm \pi/4 + \alpha, \beta)$ and $I (\pm \pi/4 + \alpha, \pi/2 + \beta)$ are measured as $\alpha$ varies from -50 to 50° with an increment of 1°, and $\beta$ varies from -0.5° to 0.5° with an increment of 0.25°. Two incident angles are taken: one is less than and the other one is larger than the principle angle; in the present case, they are 45$\pm$0.02° and 70$\pm$0.02°. A power meter (Newport 818-SL) is used as the detector. The measured intensity is digitized by a multi-meter (Keithley 195A) and is stored in PC for analyzing. A SiO$_2$/Si thin film is taken as the testing sample. The polarizer and analyzer are rotated by stepping motor of step 0.01° and 0.001° respectively.

**EXPERIMENTAL RESULTS**

According to eq. (1) and (2), we convert all the reflected intensities into intensity ratios A and B. There are two parameters can be obtained from the processes of plotting out the distribution of intensity ratios A and B with respect to $\alpha$, at a fixed $\beta$: (a) the position of intersections ($\alpha, \beta$), (b) the value of A and B at the intersection, $\tan^2 \psi$. A typical result is shown in Fig. 4. One can obtain the positions and values at the intersections of A and B by polynomial fit. Mapping out the position of intersections such as shown in Fig. 5, it is found that the incident plane is at 0.208 $\pm$ 0.004° for analyzer and 0.488 $\pm$ 0.004° for polarizer, respectively. The closest attainable scale in the laboratory for the incident plane is at $\alpha = 0.5^\circ$ and $\beta = 0.2^\circ$ such as shown in Fig. 6. Its symmetrical distribution around the incident plane for $\theta_i$ at 45° and 70° is just as expected. The value at the intersections are 1.582 $\pm$ 0.008 for $\theta_i = 45^\circ$ and 1.488 $\pm$ 0.004 for $\theta_i = 70^\circ$ respectively. According eq.(5), one can obtain $\cos \Delta$ from slope $d\beta/d\alpha$ and $\tan \psi$: at $\theta_i = 45^\circ$, $\cos \Delta = -0.946 \pm 0.012$; at $\theta_i = 70^\circ$, $\cos \Delta = 0.1331 \pm 0.012$.

**CONCLUSIONS**
In conventional null ellipsometry, the basic idea is to locate the minimum intensity for polarizer and analyzer, then use the azimuth angle of polarizer and analyzer to measure the ellipsometric parameters. A sensitive detector is essential. The intensity ratio technique is trying to release this requirement. As a standard technique for calibrating the incident plane\textsuperscript{1}, we used a marked polarizer to locate the minimum reflection of a nonabsorbing sample and consider it as the reference zero. Then, the azimuth angle of polarizer and analyzer used in this experiment are aligned to the reference zero according to the conventional technique, that is to locate the minimum transmission. All the minimums are located by a power meter. After the rough alignment, then the zeros of polarizer and analyzer are measured by intensity ratio technique. An accuracy of better than 0.005° can be achieved in this on-line measurement. $\tan^2 \psi$ revealed at the intersection is 1.582 for $\theta_1 = 45^\circ$, and 1.488 for $\theta_1 = 70^\circ$. Compared with measured values from two zone null ellipsometry, Table 1, we find that if the incident angle are corrected to be 44.82° and 69.82°, the corresponding $\tan^2 \psi$ are 1.582 and 1.489, and $\cos \Delta$ are -0.958 and 0.1433 respectively. In general, the measurement error of $\tan^2 \psi$ is smaller when $\theta_1 > \theta_p$ but the measurement error of $\cos \Delta$ is about 1% when $\theta_1 < \theta_p$. The inaccuracy of $\cos \Delta$ is expected in this PSA system\textsuperscript{8}, we are working on the PSCA system and trying to improve the measurement on $\Delta$. Without using the measurement of $\cos \Delta$, we are able to deduce the refractive index of a bulk medium within 0.2% of the published value.

ACKNOWLEDGMENTS

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REFERENCES

Table 1: Comparison between the measurement of null ellipsometry and intensity ratio technique

<table>
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<tr>
<th>Ellipsometric parameters</th>
<th>null $45^\circ$</th>
<th>Intensity ratio $45^\circ$</th>
<th>null $44.82^\circ$</th>
<th>null $70^\circ$</th>
<th>Intensity ratio $70^\circ$</th>
<th>null $69.82^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tan(\psi)^2$</td>
<td>1.588</td>
<td>1.582 (0.008)</td>
<td>1.5827</td>
<td>1.482</td>
<td>1.488 (0.004)</td>
<td>1.489</td>
</tr>
<tr>
<td>$\cos(\Delta)$</td>
<td>-0.9559</td>
<td>-0.946 (0.012)</td>
<td>-0.958</td>
<td>0.1559</td>
<td>0.1331 (0.012)</td>
<td>0.1433</td>
</tr>
</tbody>
</table>

Fig. 1 Schematic setup of the PSA ellipsometer. S: light source, HeNe laser P: polarizer, A: analyzer, D: detector.
Fig 2. Intensity ratios of A and B plotted against angular position of polarizer ($\alpha$) when the angular position of analyzer ($\beta$) is at 0° for $n=1.5$. Solid lines are the simulated theoretical curves, dotted lines are their linear approximation.
Fig. 3a The intensity ratios A and B plotted against angular position of polarizer($\alpha$) when the angular position of analyzer ($\beta$) is 2° (top), -1° (bottom) for $n=1.5$ as non-absorbing material: $\theta_i = 45^\circ$, A: dotted line B : dashed line; $\theta_i = 70^\circ$, A: thin line B: thick line. Ir : intensity ratio value.
Fig. 3b The intensity ratios A and B plotted against angular position of polarizer (α) when the angular position of analyzer (β) is 2° (top), -10° (bottom) for \( n = 0.35 - i 2.45 \) as absorbing material: \( \theta_i = 45° \), A: dotted line B: dashed line; \( \theta_i = 70° \), A: thin line B: thick line. Ir: intensity ratio value.
Fig. 4 Experimental values of intensity ratios A and B plotted against the angular position of polarizer (α) when the angular position of analyzer (β) is ±1° for a SiO₂/Si as sample. Both \( \theta_1 < \theta_p \) (\( \theta_1 = 45° \), A: ○ B: • \( \tan^2\psi = 0.1582 \)) and \( \theta_1 > \theta_p \) (\( \theta_1 = 70° \), A: □ B: ■ \( \tan^2\psi = 0.1488 \)) are measured. Ir 45: intensity ratio value for \( \theta_1 = 45° \), Ir 70: intensity ratio value for \( \theta_1 = 70° \).
Fig. 5  Angular positions of polarizer (α) and analyzer (β) where intensity ratio A = B, for \( \theta_i < \theta_p \) (\( \theta_i = 45^\circ \)) and \( \theta_i > \theta_p \) (\( \theta_i = 70^\circ \)). These two curves intersect with each other at the incident plane (\( \alpha = 0.488^\circ, \beta = 0.208^\circ \)) of SiO\(_2\)/Si thin film. The dotted (\( \theta_i = 45^\circ \)) and solid (\( \theta_i = 70^\circ \)) lines are the linear polynomial fit from the measured data.

\[ \beta = 0.2 \]

Fig. 6  Experimental values of intensity ratios A and B plotted against the angular position of polarizer (α) when the angular position of analyzer (β) is 0.2° for a SiO\(_2\)/Si as sample. Both \( \theta_i < \theta_p \) (\( \theta_i = 45^\circ \), A: O  B: ● Ir 45: intensity ratio) and \( \theta_i > \theta_p \) (\( \theta_i = 70^\circ \), A: □ B: ■, Ir 70: intensity ratio).