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A phase-stepped spectroscopic ellipsometer

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ABSTRACT

We describe a spectroscopic ellipsometer which uses a white light source and a variable wave-plate to generate four phase-stepped intensities $I(\lambda)$ which are recorded by a small spectrometer. At each wavelength, the wave-plate produces a constant, but unknown phase step $\alpha(\lambda)$. Carré's algorithm is used to determine this unknown phase step at each wavelength which subsequently allows the ellipsometric angles $\psi(\lambda)$ and $\Delta(\lambda)$ to found from the solution to a set of simple equations. We demonstrate our new instrument experimentally by measuring the retardation of an achromatic wave-plate and determining the thickness of a silicon dioxide film on a silicon substrate.

1. Introduction

Spectroscopic ellipsometry is a powerful technique that is widely used to determine the optical properties of substrates and thin films [1]. Samples are characterised by a pair of angles, ψ and Δ defined such that $\tan\psi\exp(i\Delta) = r_p/r_s$ where r_p, r_s are the (complex) Fresnel reflection coefficients of the sample. While estimates of $\tan\psi$ can be readily obtained from intensity measurements, determining Δ, which depends sensitively on film thickness, generally requires some form of modulation.

One well-established method for generating the necessary time-varying signals relies on rotating one of the elements of the ellipsometer [2–7], in which case the Fourier coefficients of the photocurrent allow one to calculate the corresponding ellipsometric angles. Another popular technique is to modulate the incident polarisation with the aid of a photoelastic modulator [8,9]. Alternatively, one can introduce a wavelength-independent phase shift and use a spectrometer to measure $I(\lambda)$ for a small number of known, fixed phase shifts. Such a phase shift can be generated using Pancharatnam's phase and we recently demonstrated an instrument based on this principle [10]. However it was essential to rotate the final polariser and the spectrometer as a single unit as the spectrometer is highly polarisation sensitive. For small spectrometers such as the USB4000 from Ocean Optics, this is not overly problematic, but it does preclude using higher resolution, bench top spectrometers.

Here we describe an instrument in which the polarisation incident on the spectrometer is constant and hence suited to any spectrometer. Since we are no longer able to use Pancharatnam's phase to generate wavelength independent phase shifts, we exploit a phase-stepping technique normally associated with interferometry [11] to generate a set of intensity measurements from which we can calculate both the (wavelength-dependent) phase shift and the ellipsometric angles. A variable wave-plate is used to produce a constant, but unknown phase step $\delta(\lambda)$ at each wavelength. Four such phase stepped intensities $I_1, \ldots, I_4$ are acquired by a spectrometer and Carré's algorithm [11] used to determine the phase step δ for each wavelength. Thereafter, a set of linear equations may be constructed from which the ellipsometric angles $\psi(\lambda)$ and $\Delta(\lambda)$ are trivially calculated.

2. Theory

A schematic diagram of our spectroscopic ellipsometer is shown in Fig. 1. Lens f_1 ensures that collimated white light is incident on a polariser P and a variable wave-plate, in this case, a Soleil–Babinet compensator (SBC). The azimuthal angle of P may be adjusted, while the SBC has its axis fixed at 0°. On reflection from the sample at some known angle-of-incidence (AOI), the light passes through a further polariser A, fixed with its axis at 45°, before being focused onto the entrance slit of the spectrometer by lens f_4.

Jones matrix algebra [12] enables us to find the electric field E_{out} at the entrance to the spectrometer:

$$E_{out} = R\left(-\frac{\pi}{4}\right)\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}R\left(\frac{\pi}{4}\right)\begin{bmatrix}r_p & 0\\ 0 & r_s\end{bmatrix} \times \begin{bmatrix}1 & 0\\ 0 & \exp(-i\delta)\end{bmatrix}\begin{bmatrix}\cos P\\ \sin P\end{bmatrix} \quad (1a)$$

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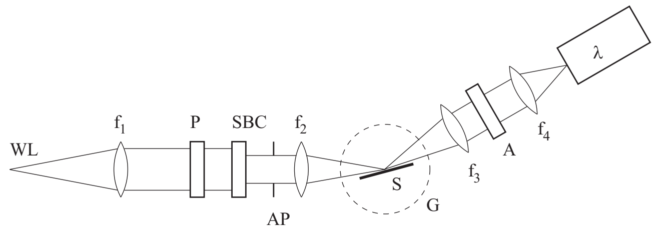

Fig. 1. Schematic of the phase-stepping spectroscopic ellipsometer. Key: WL: white light source; f_1 – f_4: lenses; P: polariser; SBC: Soleil-Babinet compensator; AP: aperture; S: sample; G: goniometer; A: analyser; λ: spectrometer.

which eventually yields

$$E_{\mathrm{out}} = \frac{1}{2}(r_p \cos P + r_s \sin P \exp(-i\delta)) \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{1b}$$

where $R(\cdot)$ is the usual rotation matrix and δ is the delay of the SBC. At each wavelength, the intensity measured by the spectrometer is therefore

$$I(\lambda,\delta) \propto r_p^2 \cos^2 P + r_s^2 \sin^2 P + 2 r_p r_s \cos P \sin P \cos(\Delta+\delta). \tag{2}$$

If the phase step δ is known, then it is possible to use any of the well established phase-stepping methods to recover the ellipsometric angle Δ [11]. In principle, it is possible to determine this phase step *a priori*. The SBC is driven by a micrometer that enables fixed phase steps to be generated merely by ensuring that the micrometer is advanced by the same amount each time. A careful measurement of the SBC phase at a single wavelength as a function of micrometer setting would be sufficient to determine $\delta(\lambda)$ since the change in optical path length is dominated by a $1/\lambda$ dependence (the wave-plate birefringence makes a negligible contribution). The sensitivity of Δ to phase stepping errors, however, depends on the algorithm chosen [11,13], with more robust algorithms generally needing more steps.

In order to make our method both completely generic and independent of such careful calibration, we use Carré's algorithm [11,14] to determine the phase step as one of the measured parameters. We acquire four phase stepped intensities, $I_1, \ldots, I_4$ and write Eq. (2) in symmetrised form as

$$I_1 = A + B\cos(\Delta - 3\delta) \tag{3a}$$

$$I_2 = A + B\cos(\Delta - \delta) \tag{3b}$$

$$I_3 = A + B\cos(\Delta + \delta) \tag{3c}$$

and

$$I_4 = A + B\cos(\Delta + 2\delta) \tag{3d}$$

where A and B represent the dc and ac terms, respectively, of Eq. (2). The phase step δ may then be calculated according to [11]

$$\delta(\lambda) = \tan^{-1}\left\{\frac{3(I_2 - I_3) - (I_1 - I_4)}{(I_1 - I_4) + (I_2 - I_3)}\right\}^{1/2}. \tag{4}$$

Writing Eq. (3d) in matrix form as $\mathbf{I} = \mathrm{M}\mathbf{c}$ where

$$\mathrm{M} = \begin{bmatrix} 1 & \cos 3\delta & \sin 3\delta \\ 1 & \cos\delta & \sin\delta \\ 1 & \cos\delta & -\sin\delta \\ 1 & \cos 3\delta & -\sin 3\delta \end{bmatrix} \tag{5a}$$

and

$$\mathbf{c} = \begin{bmatrix} A \\ B\cos\Delta \\ B\sin\Delta \end{bmatrix} \tag{5b}$$

allows the best fit values of $\mathbf{c}$ for each value of λ to be obtained in the usual way from the solution to $(\mathrm{M}^{\top}\mathrm{M})^{-1}(\mathrm{M}^{\top}\mathbf{I})$. The ellipsometric angle $\Delta(\lambda)$ is then trivially recovered from these best fit coefficients from

$$\Delta = \tan^{-1}\left(\frac{c_3}{c_2}\right). \tag{6}$$

where c_i refers to the ith component of the coefficient vector $\mathbf{c}$.

The ellipsometric angle ψ can also be retrieved from these coefficients in the following way. The fringe visibility γ is defined as

$$\gamma = \frac{B}{A} = \frac{2 r_p r_s \cos P \sin P}{r_p^2 \cos^2 P + r_s^2 \sin^2 P} \tag{7a}$$

where we have substituted appropriate expressions for A and B from Eq. (2). Using the definition $\tan\psi = |r_p/r_s|$ allows further simplification:

$$\gamma = \frac{2\tan\psi \cot P}{1 + \tan^2\psi \cot^2 P}. \tag{7b}$$

At each wavelength, the best fit coefficients $\mathbf{c}$ allow us to determine experimental values for B/A according to

$$\frac{B}{A} = \frac{\sqrt{c_3^2 + c_2^2}}{c_1}. \tag{8}$$

Eq. (7b) is a quadratic in $\tan\psi \cot P$ which is readily solved to yield:

$$\tan\psi \cot P = \frac{1}{\gamma} \pm \sqrt{\frac{1}{\gamma^2} - 1}. \tag{9}$$

Thus, given experimental values of the fringe visibility γ and a known polariser azimuth P, this equation enables us to calculate $\psi(\lambda)$. Note though, that the error in ψ due to an error in γ is unbounded as $\gamma \to 1$ which will be problematic experimentally. However, this difficulty can be completely avoided by setting P such that γ never exceeds say, 0.7 over the entire spectral range of interest.

The instrument is calibrated by placing it in the straight through configuration with air as the "sample", setting P to 45° and acquiring a set of intensities with any convenient phase step. Since we know by definition that $\tan\psi^{\mathrm{air}} = 1$ and $\Delta^{\mathrm{air}} = 0$, this enables us to calculate ψ^{cal} and Δ^{cal} for the instrument. With a sample in place, we set P appropriately and acquire another set of intensities from which we calculate the ellipsometric angles according to

$$\tan\psi^{\mathrm{sam}} = \left\{\frac{1}{\gamma} \pm \sqrt{\frac{1}{\gamma^2} - 1}\right\} \frac{\tan P}{\tan\psi^{\mathrm{cal}}} \tag{10a}$$

and

$$\Delta^{\mathrm{sam}} = \Delta - \Delta^{\mathrm{cal}}. \tag{10b}$$

Since the phase step δ is calculated afresh with each set of intensities, it is not necessary to use the same value of δ for both calibration and measurement.

3. Experimental results

The filament of a 50 W tungsten-halogen lamp was placed at the focus of a 200 mm focal length lens (f_1). The collimated light then passed through a Glan–Thompson polariser and the Soleil–Babinet compensator. Lens $f_2 = 80$ mm formed a reduced image of the filament on the sample while an aperture of approximately 4 mm diameter immediately in front of this lens limited the cone of rays incident on the sample to approximately 0.7°. The filament image was placed at the focus of f_3, a 160 mm focal length lens, so that parallel light passed through the analyser A. The final lens f_4 had a 50 mm