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ENHANCING MEASUREMENT ACCURACY IN MICROSCOPE-BASED REFLECTOMETRY FOR THIN FILM OPTICAL CHARACTERIZATION

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Abstract

Thin-film thickness characterization is important in the semiconductor and photonics industries. This study introduces for the first time an enhanced reflectance modelling method for microscope-based reflectometers with focused beams, aimed at achieving accurate thin-film thickness measurements for layers ranging from tens to thousands of nanometers. The proposed approach integrates angular distribution modelling, bandwidth correction, and thickness gradient analysis to improve the precision of modelling used to fit measured reflectance curves and extract the optical properties of the layers. Validation against a traceable gonio-reflectometer with a collimated beam shows excellent agreement across a wide thickness range, confirming the micro-reflectometer's reliability for high-accuracy, non-destructive characterization. The gonio-reflectometer's reliability was verified through an international comparison using ellipsometry method on the same samples. The advancements of this work enable more reliable thin-film analyses using microscope-based reflectometers, which offers the advantages of faster operation and suitability for measurements of small areas on semiconductor wafer samples.

Keywords: Micro-reflectometer, angle of incidence, thin film thickness, bandwidth

1 Introduction

Complex semiconductor structures require precise characterization techniques, which have increasingly favoured non-destructive methods such as reflectometry. Reflectometry, which relies on the ratio of reflected to incident light intensity, provides a fast and controllable approach for characterizing optical properties of thin films (Choi et al, 2020); (Danilenko et al, 2023). Ellipsometry is another widely used method for thin-film characterization which determines thin film optical properties by measuring the change in polarization components of the detected light (James et al, 2008).

This study investigates a microscope-based reflectometer (micro-reflectometer) featuring an on-axis focused beam incident through a microscope objective, with measurements performed on silicon dioxide (SiO₂) thin-films on silicon (Si) substrates. The novel aspects of this research include accounting for angular effects of the beam, correcting spectral bandwidth in oscillatory reflectance data, and addressing thickness gradients within the measurement area. Validation is achieved by comparing the results with those obtained from a standard gonio-reflectometer, highlighting the micro-reflectometer's capability as a traceable solution. Further indirect validation evidence is provided by an international comparison measurement with a participant using the ellipsometry method for thin-film characterization.

2 Experimental

The test samples were thermal SiO₂ layers grown on Si substrates. The uniformity of the layer thickness was controlled carefully during sample production. High uniformity of the samples is a significant advantage for reliable comparison of collimated and focused-beam measurements.

Figure 1 shows the schematic of the micro-reflectometer used for this study. Illumination was provided by halogen and deuterium lamps, with light transmitted via an optical fiber (F) and collimated by a lens (L) to the microscope compartment. The system incorporates a motorized sample stage for mapping, allowing layer-thickness uniformity analysis across the sample. Reflected light was collected by a charge-coupled device (CCD) spectrometer, and spectral reflectance data were stored in a computer. The micro-reflectometer measurements were performed in the wavelength range of 310 nm to 930 nm. The light beam was focused onto the sample using a 20x objective lens with a numerical aperture of 0,39, a focal length of 10 mm, and an entrance aperture diameter of 5,7 mm, producing a beam spot with a diameter of 200 μm on the sample. The largest angle of incidence on the sample is 15.9°.

The raw reflectance spectrum of the micro-reflectometer is relative rather than absolute. This means that determining the reflectance of the test sample requires reflectance measurement of a reference sample with a known spectral reflectance. The reference sample consists of a uniform thin layer of thermal SiO₂ on a Si substrate.

The 50/50 beam splitter (BS) and other optics used in our setup of Figure 1 are installed in a sealed, enclosed environment to minimize the introduction of dust and other contaminants that could cause additional scattering or stray light. Moreover, any stray light generated within the BS or other optics is expected to affect both the reference and test measurement equally. As a result, the influence of stray light tends to cancel out when analyzing relative measurements, thereby minimizing its effect on the final signal-to-noise ratio. Based on this configuration and environmental control, the contribution of stray light from the beam splitter is considered negligible in our system.

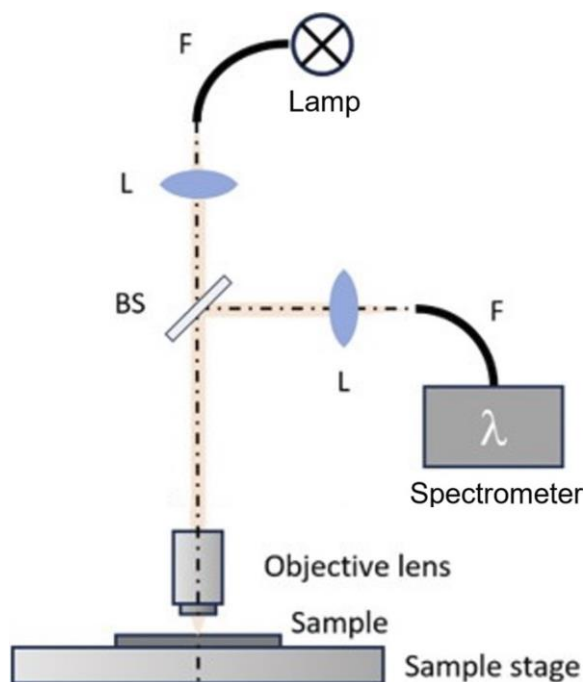


Figure 1 – Schematic of the micro-reflectometer.

Sample alignment is carried out using an external auto collimating telescope (ACT). During this process, the objective lens is temporarily replaced by an additional mirror inserted into the beam path. This configuration enables convenient observation of the measurement spot on the sample, as well as verification of the focus and tilt.

A well-characterized gonio-reflectometer with a collimated measurement beam served as a traceable instrument for validation of the micro-reflectometer results. It operates with an 11° incident angle and measures reflectance within an area on 3 mm x 3 mm across a wavelength range of 370 nm to 830 nm.

3 Theoretical Framework and Modelling

The reflectance model is derived using Fresnel equations to calculate reflection and transmission coefficients at each interface of the thin film. These coefficients account for s- and p-polarization components, enabling the formulation of a comprehensive reflectance curve with appropriate state of polarization. The model was extended to multilayer structures using the transfer matrix method (Luce et al, 2022). By fitting the modeled reflectance to the measured reflectance, we can obtain the thickness of the coated layer as one of the fitted parameters. Another fitted parameter is the width of the thickness distribution within the measurement spot, accounting for a possible gradient in the layer thickness.

In micro-reflectometry, the incident light beam forms a cone of angles, leading to a distribution of angles of incidence across the measurement area. This distribution significantly influences the reflectance curve, particularly with thicker coated layers. To account for this, the beam cone was segmented into 15 angular bands, corresponding to equidistant spatial bands in a uniform light beam incident on the objective lens. Reflectance at each angular band was weighted during the fitting process by the relative intensity within that band.

The spectral bandwidth of the spectrometer affects the reflectance curve, especially for films with pronounced oscillations in reflectance. Bandwidth correction was applied using the Richardson-Lucy method (Eichstädt et al, 2013) to improve the accuracy of thickness determination for samples with thicker coatings.

4 Results

The micro-reflectometer was employed to measure SiO₂ thin films on Si with nominal layer thicknesses of 60 nm, 512 nm, 1000 nm and 2000 nm. Figure 2 shows the measured reflectance with fitted curves and Table 1 lists the fitting results of the layer thicknesses. Accounting for the angular distribution improved the reflectance model's fit, reducing discrepancies between measured and theoretical curves. The angular distribution also influences the fitted value of the layer thickness, especially for Samples 3 and 4 with thicker coatings, where angular effects are more pronounced. Moreover, the spectral bandwidth correction also significantly impacted oscillatory reflectance curves. For thinner layer thicknesses like in Sample 1, where oscillations are minimal, the correction had negligible effects.

The micro-reflectometer results were validated against those obtained from a gonio-reflectometer, demonstrating excellent agreement across the entire thickness range. Table 1 provides the summary of the comparison between the thickness values measured by the two devices. The absolute differences between the micro-reflectometer and gonio-reflectometer measurements are small relative to the uncertainty of the measurements.

Our gonio-reflectometer participated in an international comparison measurement with another participant who used ellipsometry to determine the layer thickness of the same samples. In this comparison, for Sample 1, the absolute difference in layers thicknesses between the two methods was 1.8 nm, compared to the expanded uncertainty of 3.4 nm. For Samples 2, 3 and 4 the corresponding results were (1.0 ± 7.0) nm, (-1.8 ± 11.1) nm and (-3.2 ± 18.8) nm, respectively. The expanded uncertainties were calculated by adding in quadrature the individual expanded uncertainties from each measurement technique. With Sample 4, the large uncertainty is mainly because of the ellipsometry method. In all cases, the differences are well within the uncertainties, confirming the consistency and reliability of both methods across the tested thickness range (Rastgou et al, 2025).

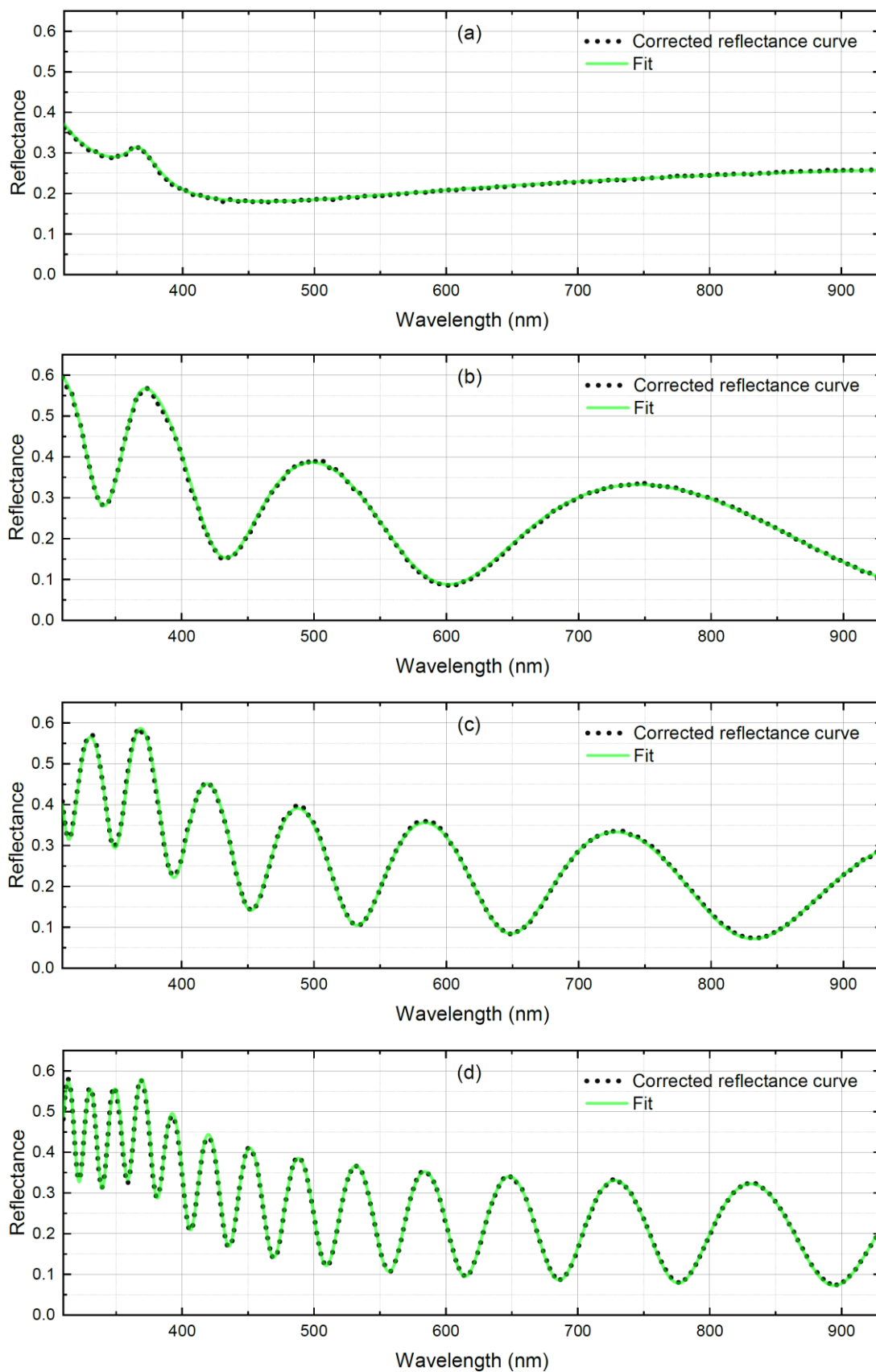


Figure 2 – Bandwidth-corrected reflectance measured with the micro-reflectometer and the corresponding fitted curve, accounting for angular incidence distribution and layer thickness variation effects for the nominally (a) 60 nm, (b) 512 nm, (c) 1000 nm, and (d) 2000 nm thick SiO₂ layer on a Si wafer.

Table 1 – Thickness measurement results for SiO₂ on Si layers obtained using a micro-reflectometer (T_{micro}) and gonio-reflectometer (T_{gonio}), including their combined standard uncertainties.

Sample	Nominal SiO ₂ thickness (nm)	T_{micro} (nm)	u_{micro} (nm)	T_{gonio} (nm)	u_{gonio} (nm)
Sample 1	60	60,3	1,7	61,0	1,4
Sample 2	512	517,6	3,3	516,4	3,0
Sample 3	1000	1007,5	4,1	1005,4	3,4
Sample 4	2000	2014,1	5,6	2008,6	4,0

5 Uncertainty Analysis

We evaluated the uncertainty in the micro-reflectometer measurements by considering several parameters. Below, we briefly describe the main factors contributing to the uncertainty of Sample 4:

- Model Sensitivity:

The sensitivity of the reflectance model to thickness variations was assessed by adjusting the fixed layer thickness during repeated fitting of other parameters. When a significant degradation in fit quality was observed, the standard uncertainty of layer thickness was calculated from rectangular probability distribution within the deviated thickness values. The standard uncertainty due to the sensitivity analysis is 2,9 nm.

- Interface Layers:

The presence of mixed layers (SiO₂/Si interface) and surface roughness (Air/SiO₂ interface) contributes to the uncertainty. Interface effects were modeled using refractive indices and thickness estimates derived from literature (Herzinger et al, 1998); (Bruggeman, 1935). The combined standard uncertainty from both interface layers is 3,6 nm, calculated by determining the difference in SiO₂ layer thicknesses when the interface layers are present versus when they are not.

Considering these uncertainty components, along with several others that had smaller effects (such as wavelength, cone angle, sample alignment accuracy, and repeatability), the combined standard uncertainty for each sample was calculated using the quadratic sum of all components. We also characterized the results obtained from our gonio-reflectometer and evaluated its uncertainty to establish a reliable basis for comparing the results from both devices. The results of uncertainty evaluation are shown in Table 1.

6 Conclusion

This study introduces an accurate modeling method based on the structure of microscope-based reflectometers for reliable and traceable thin-film thickness characterization. The combination of angular distribution modeling, spectral bandwidth correction, and thickness gradient analysis within the measurement area has enhanced measurement accuracy, validated through comparison measurements. The results showed close agreement across a wide range of thin-film thicknesses, demonstrating the method's ability to provide reliable measurements.

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