Spectroscopic Ellipsometry
Room 209 F W - Session EL-TuM

Spectroscopic Ellipsometry Analysis Methods

Moderators: Tino Hofmann, University of North Carolina at Charlotte, **Marcel Junige**, University of Colorado at Boulder

8:00am **EL-TuM-1 Crystal Symmetry and Spectroscopic Ellipsometry*, Gerald Jellison,*** Oak Ridge National Laboratory **INVITED**

Of the known crystals, over 90% are optically anisotropic and therefore birefringent.That is, the complex dielectric function depends on the polarization of the incident light and the orientation of the crystal. The general linear dielectric response for non-magnetic materials is expressed as a complex 3 x 3 symmetric tensor.This tensor can be simplified if the crystal is oriented in the laboratory reference frame, where uniaxial, orthorhombic, and monoclinic crystals require 2, 3, and 4 independent complex elements, respectively.Isotropic materials require only 1 element.Triclinic materials have no symmetry other than translation, so their dielectric tensors have 6 independent elements.

These dielectric functions are best measured by generalized or Mueller matrix ellipsometry [1].If there is no depolarization, then the ellipsometric data can be reduced to the 2 x 2 reduced Jones matrix rho where rho$_{pp}$ = rho$_{pp}$/rho$_{ss}$, rho$_{sp}$ = rho$_{sp}$/rho$_{ss}$ and rho$_{ps}$ = rho$_{ps}$/rho$_{ss}$.For isotropic materials, *rho*$_{pp}$= tan*(psi)*exp*(iDelta)*, where psi and Delta are the standard ellipsometric angles.The cross-polarization terms rho$_{sp}$ and rho$_{ps}$ will be non-zero if the coordinate system of the crystal does not match the coordinate system of the ellipsometer, defined by the plane of incidence.For uniaxial crystals, the cross-polarization terms will be zero if the optic axis is in or perpendicular to the plane of incidence.For orthorhombic and monoclinic crystals, the cross-polarization terms will be zero if a principal axis is perpendicular to the plane of incidence. Even when the cross-polarization terms are non-zero, there are some orientations of the crystal where rho$_{sp}$ and rho$_{ps}$ will be symmetric.If the optic axis of a uniaxial crystal is in the sample surface plane (Theta = 90°), then rho$_{ps}$(phi) = -rho$_{sp}$(phi), rho$_{ps}$(phi) =-rho$_{ps}$(-phi), and rho$_{sp}$(phi)=-rho$_{sp}$(-phi), where the Euler angle phi is the angle of the optic axis with respect to the plane of incidence.

This talk will discuss the symmetry relationships for uniaxial, orthorhombic, and monoclinic crystals and will show spectroscopic generalized ellipsometry data taken from several anisotropic crystals.Example crystals may include: rutile and anatase (TiO_2), ZnO, calcite and aragonite ($CaCO_3$), dolomite [$CaMg(CO_3)_2$,] zinc oxide (ZnO), tin oxide (SnO_2), andparatellurite (a-TeO_2).

[1] G. E. Jellison, Jr., N. J. Podraza, and A. Shan, “Ellipsometry: dielectric functions of anisotropic crystals and symmetry,” *J. Opt. Soc. Am*. A **39**, 2225 (2022).

8:30am **EL-TuM-3 Ellipsometric Reality Check: Are My Results Correct?*, Maxwell Junda,*** Covalent Metrology

Covalent Metrology offers a large range of analytical measurement techniques (150+) and uses these to support scientists and engineers in solving demanding problems across many different industries.There is often tremendous value in combining multiple measurement techniques on a sample to obtain complementary material property information. This provides a fuller understanding of the materials of interest.However, sometimes when spectroscopic ellipsometry (SE) is used in conjunction with other metrology, the corresponding results don’t match.This often opens a Pandora’s Box of questions about the source of the mismatch and which result is “right.”Similarly, even when evaluating ellipsometry results by themselves, the widely varying needs of each application require careful handling of how SE data is modeled and results are interpreted.

As an example, one Covalent customer is fabricating waveguides.Accuracy in our measurements of dimensions and thickness of the waveguide materials is *critically important* since these waveguides are designed to operate at a specific wavelength which defines the required dimensions.Cross sectional transmission electron micrographs (TEM) are also used to measure dimensions which, with surprising frequency, differ from best-fit SE results by a nontrivial margin.As a further complication, using TEM-derived thicknesses as fixed parameters in the SE modeling results in unacceptably poor model fits. This mismatch has necessitated investigation into properties at the interfaces that are detectable by SE, but not TEM.

By contrast, another Covalent customer is using routine SE measurements for process monitoring.Here, the repeatability of SE measurements (i.e. precision) is most important to track the deposition process over time and overall accuracy of the results is secondary.This represents a completely different use-case for ellipsometry where establishing a standardized measurement and modeling methodology for detecting deviations dominates, potentially even over accurate measurement results.

Lastly, specific choices for optical modeling configurations always have tradeoffs between physical realism, sensitivity, and practical utility.Some models are developed to accommodate gross spatial nonuniformities in films on 300mm wafers, whereas others are created to detect weak absorption modes in the infrared when paired with transmittance measurements.Although all are fundamentally based on the information encoded within SE data, the optical models used to obtain final results are unavoidably context-dependent.

8:45am **EL-TuM-4 Spectroscopic Ellipsometry Based on Frequency Division Multiplexing*, Jongkyoon Park,*** KRISS, Republic of Korea

Spectroscopic ellipsometry (SE) is a widely utilized technique in optical metrology, particularly in the semiconductor industry, for its ability to measure thin-film thickness non-destructively and with sub-nanometer precision. Various types of SE have been developed, each type offering unique strengths and limitations, making the selection of an appropriate technique crucial for specific applications. Here, we experimentally and theoretically demonstrate a novel SE technique based on frequency division multiplexing (see Fig. 1), which we call Frequency Division Multiplexing Spectroscopic Ellipsometry (FDM-SE) [1,2].

FDM-SE is a variant of traditional rotating polarizer ellipsometry (RPE) in which the broadband light source is replaced with multiple discrete-wavelength intensity-modulated laser diodes (LDs) (see Fig. 2). This modification enables obtaining the optical properties of materials at multiple wavelengths simultaneously by using a spectrally integrating detector instead of a spectrometer.

In order to assess the performance of FDM-SE method, SiO_2 films on a Si wafer with different film thicknesses were measured by FDM-SE and a commercially available conventional SE instrument. We obtain a difference between the measured thicknesses with both methods of less than 5 Å on average implying that FDM-SE can be used for accurate thickness measurements. Thus, the proposed FDM-SE technique provides a novel alternative SE approach for a variety of optical metrology applications.

9:00am **EL-TuM-5 Advanced Electromagnetic Modeling Techniques for Metamaterial Platforms*, Ufuk Kilic,*** University of Nebraska-Lincoln, USA **INVITED**

Nanostructured metamaterials play a crucial role in cutting-edge applications spanning optoelectronics, quantum information processing, and biomedical technologies [1-3]. Precise characterization of their structural and optical properties is essential for their effective integration into functional systems. The conventional spectroscopic ellipsometry (SE)-based optical characterization faces inherent limitations. SE is largely constrained to far-field analysis and relies on idealized layer-based models, making it insufficient for complex nanostructures with pronounced near-field interactions, strong nonlocal effects, and wavevector-dependent material responses.

In this talk, to overcome these challenges, we leverage the finite element modeling (FEM) based theoretical characterization, optimization, and verification technique which basically relies on the frequency dependent full-wave electromagnetic solutions of Maxwell's equation [3]. FEM provides a powerful framework for directly visualizing electromagnetic field distributions, incorporating experimental inputs from imaging techniques such as scanning electron microscopy and transmission electron microscopy, and refining optical models through spectroscopic ellipsometry-based dielectric function analysis. By enabling precise modeling of both near- and far-field interactions, as well as capturing nonlocal material responses that go beyond standard effective medium approximations, FEM pushes the boundaries of conventional characterization techniques. This deeper understanding of light-matter interactions is essential for advancing photonic, optical, and quantum materials, enabling next-generation applications.

References:

[1] Carneiro, S. V., et al., *Materials Today Nano* 22 (2023): 100345.

[2] Kilic, U., et al., *Advanced Optical Materials* (2024): 2302767.

[3]Kilic, U., et al., *Nature communications* 15.1 (2024): 3757.

9:30am **EL-TuM-7 Evaluation of Scatterometry for High Aspect Ratio Deep Trench Monitoring: A Rigorous Coupled-Wave Analysis Approach***, **Martial Santorelli**, Justine Grasland, Delphine Le Cunff,* ST Microelectronics, France*; Marceline Bonvalot,* Laboratoire des Technologies de la Microelectronique, CNRS-LTM, France*; Madec Querré,* ST Microelectronics, France*; Jean-Hervé Tortai,* Laboratoire des Technologies de la Microelectronique, CNRS-LTM, France

In the ingoing development of extreme miniaturization, gapfilling processes are truly challenged for High Aspect Ratio (HAR) 3D structures, whereby seam and void formation can occur. An in-depth characterization of such processes requires specific in-line, statistical, non-destructive and robust metrology solution, enabling accurate evaluation of filling quality. Optical scatterometry emerges as a promising technique, proven effective for characterizing empty HAR deep trench while lack of sensitivity has been shown when increasing depth and top film stack complexity [1], [2]. Scatterometry Mueller matrix formalism aptly describes the optical behavior of periodic grating structures. However, linking these matrix coefficients to physical properties remains challenging due to the variety of potentially impacting factors in complex HAR structures (film stack and geometry parameters). To overcome this limitation, Rigorous Coupled-Wave Analysis (RCWA) provides a powerful simulation framework that enables the interpretation of changes in matrix elements by leveraging the flexibility of parametric modeling combined with extensive computational capabilities [3].

Our study firstly focuses on characterizing HAR deep trenches prior to gapfilling (Figure 1a). We propose an RCWA-based methodology to analyze the influence of structural parameters, such as film thickness and trench dimensions, on key Mueller matrix elements (m_{12}, m_{33} and m_{34}). A Global Sensitivity Analysis (GSA) using Sobol indices isolating the impact of trench dimensions highlights the parameter effects in the infrared IR wavelength range. This sensitivity shifts to high IR wavelength range for deep trenches (> 4 µm), where the IR response becomes more influenced by trench slope (Figure 2). Subsequently, a comprehensive GSA including all input parameters enables model simplification by determining non-sensitive inputs from the top film stack. Instead of solving an inverse problem, experimental parameters have been extracted by selecting the closest matching response from a generated library. Gapfilling is then modeled by varying void size and position in the trench (Figure 1b-d). The rigorous pre/post gapfilling approach quantifies the influence of filling defects on the infrared spectrum while minimizing variability from other inputs. Our results demonstrate that buried voids (Figure 1c) have a slight effect on the amplitude and phase of IR oscillations, whereas partial filling (open voids, Figure 1d) significantly impacts first the frequency and then the phase in the IR range. Such defects may be detectable in the infrared spectrum when appropriate signal processing techniques are applied.

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