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 Magnetic Field-Controlled Polarized Emissivity in Low-Temperature Spin Systems via the Bloch Formalism***, **Sina Khayam,*** Mechanical and Materials Engineering Department, University of Nebraska-Lincoln, Lincoln, NE 68588*; Viktor Rindert,* NanoLund and Solid State Physics, Lund University, 22100 Lund, Sweden*; Ufuk Kilic,* Electrical and Computer Engineering Department, University of Nebraska-Lincoln, Lincoln, NE 68588*; Mathias Schubert,* NanoLund and Solid State Physics, Lund University, 22100 Lund, Sweden & Electrical and Computer Engineering Department, University of Nebraska-Lincoln, Lincoln, NE 68588

This study investigates how polarized emissivity in spin-based systems can be modulated at low temperatures using the Bloch model, focusing on the role of magnetic fields in tuning their optical response. The emissivity, a key quantity in radiative heat transfer, is strongly influenced by the temperature-dependent distribution of spin states, which in turn is governed by their interaction with magnetic fields. To model this, we use a permeability tensor derived from Bloch's equations for nuclear magnetic moments in magnetically resonant materials [1, 2, 3], combined with a dielectric permittivity tensor. These tensors are incorporated into a 4×4 matrix formalism [4] to compute emissivity and analyze how its polarization properties are affected by magnetic anisotropy. The study also presents a generalized analytical framework for calculating thermal emissivity that accounts for both magnetic and dielectric responses under varying temperature and magnetic field conditions. Model validation is performed using WVASE32TM ellipsometry software, confirming the accuracy of theoretical predictions. Overall, this work provides new insights into magnetically tunable quantum emissivity, with promising implications for next-generation thermal management in quantum and nanoscale technologies.

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