Spectroscopic Ellipsometry
Room 320 - Session EL-ThA

Spectroscopic Ellipsometry Oral Session

Moderators: Dr. Andy Antonelli, Antonelli Research and Technology, **Dr. Ufuk Kilic**, University of Nebraska - Lincoln, **Dr. Nikolas Podraza**, University of Toledo, **Prof. Dr. Eva Schubert**, University of Nebraska - Lincoln

2:15pm **EL-ThA-1 Spectroscopic Ellipsometry for Advanced Semiconductor Metrology Applications***, **Matthew Hilfiker**, Rostislav Grynko, Nick Keller,* Onto Innovation **INVITED**

Advanced logic and memory development continues to push device architecture well beyond the limits of traditional process control methods. As dimensions shrink and structures become increasingly complex, parameter correlation has increased, placing new demands on both metrology sensitivity and model robustness. While spectroscopic ellipsometry has long been a workhorse technique in semiconductor manufacturing, its effective use at advanced nodes requires broader spectral coverage, improved modeling approaches, and tighter control of measurement uncertainty.

This talk provides an overview of spectroscopic ellipsometry as it is applied to today's most challenging metrology problems. Measurements in the visible and ultraviolet remain critical for monitoring dimensional control at the atomic scale. At the same time, mid–infrared ellipsometry has emerged as an important complement, offering enhanced sensitivity to structural effects that are difficult to access at shorter wavelengths. Together, these capabilities allow metrology strategies to be tailored to the specific physics and correlations of a given process step.

As device architecture continues to evolve, improving metrology performance increasingly depends on combining advanced optical modeling with measurement approaches that remain stable across highly correlated parameter spaces. The role of rigorous coupled physical wave analysis (RCWA) enabling optical critical dimension analysis of complex three–dimensional structures will be discussed. The presentation will emphasize broader trends shaping spectroscopic ellipsometry as a critical enabler of advanced semiconductor manufacturing.

2:45pm **EL-ThA-3 In It to Thin It: Spectroscopic Ellipsometry for Native Oxide Measurement on Indium Thermal Interface Materials***, **Maxwell Junda**, Biswas Subedi,* Covalent

Native oxide layers on metal surfaces critically impact performance across industry. In semiconductor advanced packaging, native copper oxide at Cu-Cu hybrid bond interfaces can inhibit both electrical connectivity and bond integrity. For batteries, oxide on current collector foils influences interfacial impedance, and, for medical implants, surface oxide on titanium dictates biocompatibility and corrosion resistance. Here, we present the case of indium-based thermal interface materials (TIMs) where native oxide degrades wetting, thermal, and mechanical properties at the bond interface, contributing to void formation during reflow. Excessive oxidation can ultimately lead to thermal hot spots and reduced device reliability, making oxide thickness a key quality metric.

There are only a few metrology options for native oxides on metals. Being non-destructive, fast, and compatible with production inspection workflows makes spectroscopic ellipsometry (SE) appealing. The reality is, however, that topography, grain structure, and oxide composition variability on production surfaces present challenges for SE. Additionally, accuracy requires managing correlation between the oxide thickness and optical properties of both the metal and oxide in the optical modeling.

Covalent has developed a reliable SE-based native oxide thickness measurement on indium TIM surfaces. To overcome the inherent variability of commercial indium surfaces, we collect many distributed individual measurements to yield statistical distributions of oxide thickness. This ensures that locally anomalous sites do not overly bias the representative characterization of the overall oxidation level. Optical constants for both the indium metal and its native oxide were established through simultaneous multi-sample fitting across samples of varying oxidation, producing a robust model in which only oxide thickness remains as a fit parameter for routine inspection. Results were validated against both cross-sectional TEM and XPS. Oxide thicknesses for minimally oxidized samples are typically on the order of 5 nm. We also applied this methodology to compare as-received to intentionally oxidized samples, successfully discriminating oxide thicknesses relevant to TIM quality control. TIM shelf life was also studied through repeated measurements over time. This methodology is now deployed for routine indium TIM inspection.

Finally, we will discuss plans to extend this work with imaging ellipsometry to investigate oxide thickness variation at the microscale, to understand how surface topography and grain boundaries contribute to the spatial variability observed in focused-spot SE measurements.

3:00pm **EL-ThA-4 Developing an Optical Database of Thermally Evaporated Cadmium Selenide Telluride Alloys for Machine Learning Enhanced Spectroscopic Ellipsometry***, **Alex Bordovalos**, Nadeesha Katakumbura, Eva Mulloy, Bishal Shrestha, Suresh Chaulagain, Marie, Solange Tumusange, Balaji Ramanujam, Randy Ellingson, Ambalanath Shan, Nikolas Podraza,* University of Toledo

Machine learning techniques have shown great promise for performing rapid spectroscopic ellipsometry data analysis on simulated ellipsometric spectra in select case studies. It is critical that machine learning enhanced spectroscopic ellipsometry (MLSE) is applied to measured ellipsometric spectra collected for samples with varieties of layer structures to demonstrate its utility while developing a better understanding of transitioning MLSE from simulated ellipsometric spectra to measured ellipsometric spectra. To this end,the complex dielectric function (ε = ε1 + iε2) spectra of thermally evaporated cadmium selenide telluride (CdSe(x)Te(1-x)) alloys are established for the purpose of simulating ellipsometric spectra that represent current fabrication techniques in CdSe(x)Te(1-x) photovoltaic (PV) devices.

A series of ten thermally evaporated CdSe(x)Te(1-x) alloys are deposited on commercial transparent conducting oxide glass. These alloys are measured with energy-dispersive X-ray spectroscopy to have Se content (x) of 0.00, 0.14, 0.25, 0.31, 0.36, 0.46, 0.62, 0.75, 0.85, and 1.00. A cadmium chloride (CdCl2) heat treatment, standard to PV devices, is applied to the alloys which are then measured with X-ray diffraction to reveal a wurtzite crystal structure at x ≥ 0.62 and a zinc blende crystal structure at x ≤ 0.46. Spectroscopic ellipsometry measurements are performed on these alloys. ε2 is determined using a background TaucLorentz oscillator, an Urbach tail, and a series of excitonic critical point parabolic band oscillators with common phase for a given crystal structure while ε1 is determined from analytically solving Kramers-Kroning integration and a Sellmeier expression. A set of polynomial fits are then applied to each optical property parameter to establish the variations of each parameter as a function of Se content. These relationships reduce the number of model fit parameters by mapping these optical property parameters to x.

This optical model for CdSe(x)Te(1-x) alloys is well suited for simulating ellipsometric spectra for the purposes of developing MLSE for CdSe(x)Te(1-x) PV applications because it has a comparatively smally number of parameters and the model generated optical properties are representative of materials in current devices. The next steps include training an MLSE model using simulated ellipsometric spectra and then applying the MLSE to measured ellipsometric spectra collected from CdSe(x)Te(1-x)PV device stacks.

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3:15pm **EL-ThA-5 Spectroscopic Ellipsometry Studies of Materials for High Power Electronics***, **Madan Kumar Mainali**, Prabin Dulal, Bishal Shrestha, Suresh Chaulagain, Venkanna Kanneboina, Ambalanath Shan, Nikolas Podraza,* University of Toledo

Wide band gap materials 4H-SiC and 6H-SiC are two hexagonal crystal polytypes of silicon carbide. It is used in high power electronics as it has high thermal conductivity, high operational temperature, higher efficiency with lower power loss, and high switching frequency. Spectroscopic ellipsometry is used to characterize the optoelectronic properties of 4H-SiC and 6H-SiC (0001) single crystal samples from MTI Crop, over the infrared (IR) to vacuum ultraviolet (VUV) (0.05 – 8.5 eV) spectral range. Spectroscopic ellipsometry is a non-contact optical characterization technique sensitive to structural (bulk film thickness, interfacial layer thickness, surface layer thickness), optical properties (band gap, above band gap transitions, phonon modes), and electronic transport (resistivity, carrier concentration, carrier mobility, scattering time, and carrier effective mass) properties. Complex dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) spectra are obtained from reflection mode spectroscopic ellipsometry for backside roughened 4H-SiC and 6H-SiC. A single parametric model describing ε predominately for the ordinary directions is developed over the 0.05 – 8.5 eV for 4H-SiC and 6H-SiC with some contribution from the extraordinary direction of 6H-SiC in the IR region. Indirect band gaps for 4H-SiC and 6H-SiC are found to be 3.30 and 3.03 eV, respectively, and the corresponding direct optical gaps are at 4.46 and 4.42 eV. A model describing the optical response in the IR spectral range is created using a Drude expression with either transverse optical (TO) and longitudinal optical (LO) (TOLO) or Lorentz oscillator models. Free carrier concentration (*N*) is optically measured to be 3.7 × 10^{18} and 3.3 × 10^{18} cm^{-3} using TOLO and Lorentz oscillator models respectively, and the corresponding carrier mobility (μ) is 34 and 39 cm^2/Vs for 4H-SiC. For 6H-SiC, *N* is measured to 8 × 10^{18} cm^{-3} using either TOLO or Lorentz oscillator models and μ in the ordinary direction is 9 and 10 cm^2/Vs using the TOLO and Lorentz oscillator model, respectively, and 5 cm^2/Vs in the extraordinary direction using either model. For 4H-SiC, using the TOLO oscillator model, TO and LO phonon modes are obtained at 797.7 and 992.1 cm^{-1}, respectively. In 6H-SiC, TO modes in ordinary and extraordinary directions are found at 797.7 and 789.7 cm^{-1} and the corresponding LO modes are found at 992 and 984 cm^{-1}, respectively. The TO and LO modes obtained from the Lorentz oscillator model are consistent with modes obtained from TOLO model.

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3:30pm **EL-ThA-6 Photoacoustic Simulations for Acoustic Critical Dimension Metrology***, **George Antonelli**,* Antonelli Research & Technology*; Brian Daly,* Vassar College

Picosecond laser ultrasonics is a twenty year old high volume semiconductor metrology and continues to find new applications. One of the strengths of this technique is the deep connection between the development of the hardware and the multi-physics simulations that allow the extraction of critical parameters. As semiconductor devices continue their shift from 2D to 3D, analysis of photoacoustic data has become more challenging as the simulations are in general limited to planar stacks of films. The development of fast numerical methods for solving 3D light-matter interactions enabled the leap from films to structures giving birth to optical critical dimension (OCD) metrology.These numerical tools offer a template for a similar leap in photoacoustics. Acoustic critical dimension (ACD) metrology like OCD is an optical method, but it can non-destructively extract critical dimensions of 3D structures buried beneath an opaque surface. This method requires a new class of multi-physics simulation capable of performing tightly choreographed optical, electronic, and coupled opto-mechanical calculations. In this paper, previous work on this topic will be summarized and new algorithms realized in a software package under development will be presented. Two key components of this work are (1) the democratization of this complex analysis to facilitate its use by undergraduates and (2) a shift away from the structure definition as geometry found in OCD today and towards a process driven paradigm. Structures are therein defined by the way they are manufactured and fits on the structures can be linked back to the fundamental process parameters.

3:45pm **EL-ThA-7 Optical Modeling of Plasmonic Nanostructures***, **Peter Petrik**, Géza Szántó, Deshabrato Mukherjee, Chao Zeng, Máté Stift, Shayesteh Raeisi, Zoltán Lábadi,* Centre for Energy Research, Hungary*; Attila Bonyár,* Budapest University of Technology and Economics, Hungary*; Miklós Fried,* Centre for Energy Research, Hungary

Plasmonic nanostructures are utilized in many applications for sensing, photonics, and much more. General models in ellipsometry that focus on transfer matrix, effective medium, first principle oscillators, and analytical dispersion functions show difficulties when modeling such structures. In this work we present modeling approaches and applications for characterizing a broad variety of plasmonic and periodic nanostructures, including gratings, nanoparticles created by annealing, electrochemistry, as well as combinatorial sputtering. The formation of nanoparticles was monitored during annealing and electrochemistry. We utilized both through-liquid and Kretschmann-Raether cells for monitoring the growth of gold layers in an electrochemical cell, as well as the interaction between silk layers and analytes in Kretschmann configurations. We also studied the adsorption of flagellar filaments on nanostructured gold surfaces and their electrochemical sensing performance. The optical sensing properties of periodic gold nanostructures were also investigated in terms of measuring the ambient and thin overlayers, as well as the sensitivity for the determination of the dimensional parameters of the periodic structures. Using simplified hemispherical numerical models, we explained the sensing performance of annealed gold layers created by combinatorial sputtering. The sensitivity as a function of the initial amount of deposited gold and type of analyte was measured and explained by numerical finite element modeling of the gold nanostructures and adsorbed layers.

4:00pm **EL-ThA-8 Engineering Anisotropic Optical Properties in Hybrid Plasmonic Metamaterials***, **Ufuk Kilic**, Raymond Smith, Yousra Traouli,* University of Nebraska-Lincoln*; Christos Argyropoulos,* Pennsylvania State University*; Eva Schubert, Mathias Schubert,* University of Nebraska-Lincoln

Hybrid plasmonic metamaterials provide a powerful platform for tailoring light–matter interactions through structural control of their effective dielectric properties [1-3]. Here, we investigate the anisotropic optical response of bottom-up engineered Si–Ag hybrid plasmonic metamaterials fabricated using glancing angle deposition (GLAD). Sequential oblique-angle depositions combined with controlled substrate rotation enable deterministic control of nanocolumn geometry, optical anisotropy, and structural handedness over large areas [2-3]. The optical properties are characterized using Mueller matrix generalized spectroscopic ellipsometry (MM-GSE) from the near-infrared to the ultraviolet spectral range. Multi-layer anisotropic effective-medium approximation analysis is employed to extract the wavelength-dependent dielectric tensor elements and quantify the influence of plasmonic–dielectric hybridization on the effective optical response. The extracted dielectric functions reveal pronounced anisotropy and strong tunability arising from the engineered morphology, material composition, and structural handedness of the nanocolumn architectures.

Finite-element-method simulations are performed to establish the physical origin of the observed optical behavior. The simulations reveal strong polarization-dependent field localization and spin-dependent plasmonic mode coupling, producing enhanced optical anisotropy and broadband chiroptical activity, including pronounced circular dichroism extending from the near-infrared to the ultraviolet. Excellent agreement between experiment and theory validates the extracted dielectric functions and effective-medium analysis. **Complementary high-resolution imaging, crystallographic analysis, and compositional characterization, including scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD), confirm the formation of spatially coherent, compositionally distinct, and morphologically uniform hybrid nanocolumn arrays.**The combined experimental and theoretical investigation establishes a framework for engineering anisotropic dielectric functions in hybrid plasmonic metamaterials through nanoscale structural design. The demonstrated tunability of the effective dielectric response provides opportunities for polarization-selective photonics, broadband chiral platforms, optical sensing, and integrated nanophotonic technologies.

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.

4:15pm **EL-ThA-9 From Disordered Nanoparticles to Periodic Gratings: A Unified Framework for High-Precision Plasmonic Metrology***, **Deshabrato Mukherjee**, Géza Szántó, Chao Zeng, Máté Stift, Shayesteh Raeisi, Zoltán Lábadi,* Centre for Energy Research, Hungary*; Attila Bonyár,* Budapest University of Technology and Economics, Hungary*; Miklós Fried, Peter Petrik,* Centre for Energy Research, Hungary

We developed a high-throughput screening and ultra-sensitive detection framework using two distinct architectures: a disordered graded gold nanoparticle platform for rapid process optimization and periodic gold gratings for predictable accurate performance.

The high-throughput combinatorial platform was created by depositing graded gold layers (0-20 nm) along the X-axis on fused silica using magnetron sputtering, followed by annealing up to 600°C. This led to the formation of self-assembled nanoparticles with laterally varying surface density from 2090 to 88 particles/μm^2, resulting in an evolution of morphology from oblate to hemispherical. This was followed by spatially resolved operando tracking using a modular Avantes fiber optic scanning spectroscopy system that mapped the transition of the localized surface plasmon resonances and volatile vapor pathways. The finite element method (FEM) calculations were modeled using JCMsuite to analyze nanoparticle formation and near-field properties. To detect ethanol, water layers via Peltier cooling, and chemisorbed MBA monolayers, we isolated specific thickness thresholds from 1.6 to 3.2 nm as the optical sensing regimes. These findings were evident due to the localized geometry and the near-field coupling due to the inter-particle gaps resulting in a surface-enhanced Raman spectroscopy (SERS) enhancement factor of 10^6 under confocal laser excitation.

Complementing this, we developed periodic gold gratings using a non-destructive metrology framework. The periodic gold gratings (CD between 70-130, thickness 60 nm, and period 200 nm) were fabricated using electron-beam lithography and reactive ion etching. These grating parameters were chosen for fabrication after multi-dimensional FEM simulations using JCMsuite to determine the changes or variations in the amplitude ratio represented by Ψ and the phase difference represented by Δ of the polarized reflection coefficients. The gratings were measured in reflection-mode with Woollam M-2000DI spectroscopic ellipsometer and fitted, and complemented with FEM modeling that enhances the traditional effective medium approximations. We demonstrated that the phase-sensitive parameter, Δ, provides superior sensitivity over the amplitude parameter, Ψ simulating across a five-dimensional parameter space that included the critical dimensions, period, thickness, wavelength, and angle of incidence. Using structural partial derivatives, we achieved a bulk refractive index limit of detection of 10^{-5} refractive index units, a critical dimension uncertainty in the picometer range, and a surface mass density limit of detection of 10 pg/mm^2 using De Feijter overlayer modeling.

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