Spectroscopic Ellipsometry
Room Ballroom A - Session EL-ThP

Spectroscopic Ellipsometry Poster Session

EL-ThP-1 Optical Properties of Metal Thin Films Measured by Spectroscopic Ellipsometry, ***Kathryn Brown**, Suresh Chaulagain, Prabin Dulal, Mohammed Alaani, Ambalanath Shan, Nikolas Podraza,* University of Toledo

As the race for higher and higher efficiency photovoltaic (PV) cells accelerates, device simulation has gone from a niche theoretical tool to an absolute necessity. In order to make these simulations as accurate as possible, it is vital to have well understood optical properties for each layer in the device. One such layer which is often overlooked is the metal back contact.

This work investigated the optical properties of three common back contact materials, namely Copper, Silver, and Gold. Thin films of each metal were deposited on fused silica glass. All three films studied were of a nominal thickness such that they appear functionally infinite to the instrument. Samples were measured by variable angle spectroscopic ellipsometry (VASE) in the range from 0.031-5.87 eV and at three separate angles of incidence, 50°, 60°, and 70°. Data from two separate instruments were combined to achieve this range. The resulting data were analyzed using the Sellmeier method to create Kramers–Kronig consistent parameterized models for each material. Properties interpreted from these results include complex refractive index ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) and surface roughness.

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EL-ThP-2 Engineering the Optimal Filter: Nonlinear Noise-Reducing Filters in Spectroscopy, ***David Aspnes**,* North Carolina State University; *Long Le,* Vietnam Academy of Science and Technology, Viet Nam; *Young Kim,* Kyung Hee University, Republic of Korea

In previous work, we assessed linear filters used in spectroscopy, which operate by attenuation. Here, we assess nonlinear filters, which operate by replacement. By eliminating apodization errors, these nominally outperform linear filters but require some level of modeling. In direct (spectral) space (DS) this takes the form of replacing all or part of the data with least-squares-fit model lineshapes. In reciprocal- (Fourier-) space (RS), the equivalent is least-squares-fitting model coefficients to the low-order coefficients dominated by information, then replacing the higher-order data coefficients dominated by noise. The RS approach is new, and required appropriate mathematical functions to be developed. This generalizes RS filtering, because the only previous approach, the corrected-maximum-entropy (CME) method, can be applied only to spectra that are positive-definite and have no dispersion character. In RS filtering the option also exists to retain some of the low-order data coefficients, an advantage for complicated spectra.

Using false-data calculations, we rank filters in order of performance. If a model is known to represent a spectrum accurately, the best filters are DS lineshape-fitting and its RS counterpart. The next best are the partial-replacement RS noted above, and, in situations where it can be applied, the CME. As expected, apodization errors relegate linear filters to last place, although they have the advantages of simplicity and not requiring modeling.

Finally, our calculations show unequivocally that the fundamental limit of any filter, linear or nonlinear, to extract information from spectra is the inability to separate information from low-order noise. Examples are provided.

EL-ThP-3 Optical Properties of CrN Measured by Spectroscopic Ellipsometry, ***Farihatun Jannat Lima**, Alexander Bordovalos, Suresh Chaulagain, Ambalanath Shan, Nikolas Podraza,* University of Toledo; *Dilara Sen, Olivia Fairlamb, Frank Peiris,* Kenyon College; *Duc V. Dinh, Xiang Lü, Oliver Brandt,* Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

Chromium nitride (CrN), a transition-metal nitride, has attracted attention in the field of electronics and energy as resistive coatings due to its excellent mechanical characteristics. It also has intriguing electronic, magnetic, and thermoelectric properties. In this work, an epitaxial (111) oriented CrN film deposited on Al2O3 (0001) is measured by spectroscopic ellipsometry over a spectral range from 0.031 to 5.877 eV to extract complex optical properties and bandgap energy using a rotating compensator Fourier transform infrared (IR) ellipsometer (FTIR-VASE, J.A. Woollam Co.) and a single rotating compensator multichannel ellipsometer (J.A. Woollam Co. M-2000) from the near IR to ultraviolet. Divided spectral range analysis is performed to determine structural parameters and thicknesses and initial sets of optical properties described by physically realistic models in the respective spectral ranges. The weakly absorbing photon energy range from 0.3 to 0.734 eV is initially ignored to prevent model-dependent bias in the vicinity of the bandgap. From the structural model, it is determined that CrN surface is optically less dense than the bulk of the thin film. Numerical inversion is performed over the full measured spectral range to determine the complex dielectric function (ε = ε1 + iε2) spectra of CrN. The numerically inverted ε spectra in the full measured range is parametrized using a Kramers-Kronig consistent model. Three transverse optical (TO) phonon modes are observed at 387 cm-1, 403 cm-1 and 1048 cm-1. Three corresponding longitudinal optical (LO) phonon modes are identified from the loss function (−1/ε) at 596 cm-1, 622 cm-1 and 871 cm-1. The absorption coefficient (α) is determined from numerically inverted spectra in ε. Tauc plots of (αhv)2 and (αhv)1/2 as functions of photon energy reveal a direct gap energy of 0.815 eV and an indirect gap energy of 0.56 eV.

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EL-ThP-4 Optical and Structural Properties of Sbxsey Thin Film Co-Evaporated via Elemental Sources, ***Bishal Shrestha**, Mohammed Razooqi Alaani, Madan Mainali, Alisha Adhikari, Balaji Ramanujam, Prabin Dulal, Venkanna Kanneboina, Ambalanath Shan, Nikolas Jacob Podraza,* University of Toledo

Antimony selenide (Sb_2Se_3) is low cost, highly stable, low toxicity, high radiation tolerant, and earth abundant semiconductor with established applications in photodetectors, batteries, and memory device technologies. In recent years, it has emerged as a promising photovoltaic absorber owing to its high visible light absorption coefficient (>10^5 cm^{-1}), quasi one-dimensional structure favoring charge transfer, and an optimal band gap (1.1 – 1.3 eV). Although the current record power conversion efficiency for a single-junction Sb_2Se_3 solar cell stands at 10.57% with a theoretical limit of ~32%, further performance gains are primarily limited by the persistent challenge of achieving high-quality, phase-pure, and stoichiometric Sb_2Se_3 thin films. Owing to substantial disparity in vapor pressures between Sb and Se during deposition, conventional chemical and physical deposition techniques requiring precursor Sb_2Se_3compounds result in thin films with compositional deviations, secondary phases, and elevated defect densities, requiring additional treatments to lower the degree of imperfections. Hence, for photovoltaic device applications, an ideal fabrication and characterization technique must be developed to obtain optimized films with the appropriate optical, structural, morphological, and compositional properties. With this motive, our approach employs thermal co-evaporation of elemental Sb and Se sources, enabling improved stoichiometric control of Sb_xSe_y thin films through independent regulation of source temperatures. For material characterization, particular emphasis is placed on in-situ and ex-situ spectroscopic ellipsometry analysis to investigate evolution of optical response and structural parameters in the as-deposited to post-deposition annealed states of the films. Our study of complex dielectric function spectra over an extended spectral range from 0.03 eV (mid-infrared) to 5.87 eV (ultraviolet) is the first documented experimentally derived data for this material. These comprehensive optical data will serve as valuable resource for device simulation across broad spectral range to explore material's further potential, whereas the optical/structural parametric expression developed here can be applied to investigate similar materials regardless of fabrication technique. Scanning electron microscopy, energy dispersive spectroscopy, and x-ray diffraction measurements are used to compare the morphological, compositional, and crystallographic characteristics of the as-deposited and annealed thin films.

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EL-ThP-5 Composition-Dependent Optical Properties of Silver-Aluminum Alloy: An Ellipsometric Approach, *Jonas Sikah, **Will Cusak**, Alexander Kozen, Matthew White,* University of Vermont

Semitransparent metal thin films have been widely used in optoelectronics because of their excellent optical and electrical properties. Among such, silver (Ag) is commonly employed due to its excellent conductivity and low optical losses in the visible range. In addition, introducing a minor fraction of Al into Ag facilitates the formation of smooth thin films by decreasing the percolation threshold of pure Ag. However, the optical properties of these Ag-Al alloy films fails to represent the weighted average of optical properties of their independent metal counterparts. Therefore, we present a detail ellipsometric investigation of the optical properties of Ag-Al alloy thin films deposited on glass substrates using vacuum thermal evaporation. The alloy compositions were tailored by adjusting deposition rates to achieve Ag volume fractions ranging 100% to 0% while Al volume fractions ranging from 0% to 100%.The film thicknesses of all compositions of Ag-Al alloys were kept at 100 nm. Scanning electron microscope (SEM) images confirmed the smooth film formation when Al content is higher in the alloy film. Energy-dispersive X-ray spectroscopy confirmed the compositional variation, with atomic percentages tracking the intended volume fraction. Spectroscopic ellipsometry was conducted at room temperature across 200 – 1000 nm at incident angles of 500, 550, and 600. The complex refraction index (*n*) and dielectric function (*k*) were extracted using model-based fitting employing Bruggeman effective medium approximations.Within the UV–Visible spectral range, increasing the Ag concentration resulted in a reduction of *n* values, while a progressive increase in Al content led to an enhancement of *n* in Ag–Al alloy thin films. At near-IR to IR region, films with higher Ag content exhibited higher *n* values while increasing Al content systematically reduced the *n* values exhibiting a trend typical of metallic films due to the decreasing contribution of free electrons response. The *k* values followed a constant trend thoughtout the UV-Visible-IR range with a lower *k* values with higher Ag content and higher *k* values with lower Ag content in the Ag-Al alloy. These findings demonstrate the tunablity of optical behavior linked to alloy compositions which can be applied to plethora of optoelectronic devices accordingly.

EL-ThP-6 iCVD Parameters with Structural and Dielectric Properties of Hydrophobic and Hydrophilic Polymer Thin Films: A Multi-Sample Spectroscopic Ellipsometry Analysis*, **Parvez Amin Khan**, Hamidreza Mohajeri, Ufuk Kilic,* University of Nebraska - Lincoln*; Mathias Schubert,* University of Nebraska-Lincoln*; Siamak Nejati,* University of Nebraska - Lincoln

Unlike the conventional Chemical Vapor Deposition (CVD) process, initiated CVD (iCVD) offers a unique, solvent-free pathway for synthesizing conformal polymeric thin films. Their tailored chemical functionality such as hydrophilicity, hydrophobicity, and lipophobicity polymer thin films have been utilized in several technological applications including photocatalytic applications, sensors, organic LED, and solar cells. In this study, we provide a comprehensive investigation on the wettability characteristics of iCVD grown Polytetrafluoroethylene (PTFE) and poly glycidyl methacrylate (pGMA) thin films. We focused on their hydrophobic and hydrophilic performances and correlated them to their optical and material properties. The pGMA and PTFE thin film samples were fabricated at 350°C on silicon wafer with a deposition rate of 7.89 nm/min and 8.26 nm/min respectively. The relationship between deposition parameters (filament temperature, monomer flow rates) and material and structural properties of fabricated thin films (thickness, roughness, surface energy) were identified using spectroscopic ellipsometry techniques, X-ray photoelectron spectroscopy and the wettability characteristics of fabricated thin films were extracted from contact angle (CA) measurements. Moreover, Multi-Sample Approach based spectroscopic ellipsometry data analysis provides the dielectric function of the fabricated films across the near-infrared (0.72 eV) to vacuum ultraviolet (6.4 eV) spectral range. Cauchy dispersion model with Urbach absorption tail is employed for extracting parametrized optical properties of thin films. We found that while the optical properties remain identical for different thickness of the fabricated polymers, we observed an increase in the roughness from 21.97nm to 38.04nm with the increase in thickness from 29.32nm to 123.86nm of the thin films. For PTFE, the increase in roughness also results in enhanced hydrophobic characteristics as we observed 18% increase in the CA of drop cast DI water with increase in the thin film thickness. For pGMA, we also increase the thickness from 95nm to 118nm, however the roughness layer thickness was not changing. From the CA measurements, we found that unlike pTFE, pGMA exhibit hydrophilic characteristics and the increase thickness did not change wettability due to the surface morphology remain unchanged and the constant surface energy profile of this polymer kind. This finding shows the importance of surface profile in wettability characteristics of thin films which are critical in the advancement of surface engineering pathways.

EL-ThP-7 Optical Properties of Boro-aluminosilicate Glass using Spectroscopic Ellipsometry from 0.079 to 5.89 eV*, **Eva Mulloy**, Prabin Dulal, Suresh Chaulagain, Emily Amonette, Alex Bordovalos, Ambalanath Shan, Nikolas Podraza,* University of Toledo

Boro-aluminosilicate glass has high mechanical strength and chemical durability and is used widely in a variety of applications, including liquid crystal display substrates, glass fibers, thermal shock-resistant glass containers, and radioactive waste glasses. A commercially available boro-aluminosilicate glass is optically characterized by reflection mode spectroscopic ellipsometry and unpolarized transmittance over the infrared (IR) through the ultraviolet (UV) spectral range. Ellipsometric spectra (N, C, S) are collected using a near IR to UV rotating compensator spectroscopic ellipsometer from 0.73 to 5.89 eV (M-2000FI, J. A. Woollam Co.) and one further extended in the IR from 0.032 to 0.73 eV (IR-VASE, J. A. Woollam Co.) each at 50°, 60°, and 70° angles of incidence. A continuous parameterization of complex dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) spectra is developed from 0.079 to 5.8 eV. The parameterization of ε for this glass consists of a constant additive term to ε_1 (ε_∞), a Sellmeier expression, and Gaussian oscillators. A transfer-matrix-based numerical inversion of unpolarized transmittance spectra provides enhanced sensitivity to weak absorption from the UV to the near IR region. Parameters defining absorption features in numerically inverted ε_2 are fixed, and parameters only impacting ε_1 are fit to produce a final parametric model. From ε, distinct infrared vibrational modes can be linked to specific bonding configurations, while the onset of ultraviolet absorption arises from electronic transitions and defect states within the glass network. Sensitivity to relatively strong features at 1379, 1040, 745, and 332 cm $^{-1}$ is obtained from ellipsometry, and transmission can resolve weaker features at 1782, 2710, and 3541 cm^{-1}.

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EL-ThP-8 Birefringence of GdScO3 using Transmission Spectroscopic Ellipsometry*, **Prabin Dulal**, Balaji Ramanujam, Nikolas Podraza, Ambalanath Shan,* University of Toledo

Gadolinium scandate ($GdScO_3$) is an emerging material with potential applications in advanced electronics and photonics primarily due to its interesting electronic, magnetic, and optical properties. It crystallizes as a perovskite-type oxide with an orthorhombic crystal structure, exhibiting a high dielectric constant, thermal stability, and large band gap energy. This study investigates the optical properties of a commercially available single crystal, double-sided polished $GdScO_3$ sample with a (110) Miller index surface plane orientation. The birefringence of the sample was derived using Mueller matrix spectroscopic ellipsometry (SE) over a spectral range of 280 nm to 1650 nm.

A full set of Mueller matrix data were obtained using an ellipsometer in straight-through mode with the sample at normal incidence. The fast axis of the biaxial sample was aligned with respect to the transmission axis of the polarizer in the generation arm of the ellipsometer. The measured matrix elements show no discernible dichroic effects, and the off-diagonal elements are virtually zero, implying that the sample exhibits properties of an ideal compensator. The measured lower right block Mueller matrix element data, composed of pure sinusoidal functions of retardance, shows oscillatory behavior with respect to spectra, consistent with a compensator with high retardance due to the thick (~ 0.54 mm) sample being evaluated. The lower right matrix elements also show a steady attenuation in the oscillatory data, beginning around 600 nm and approaching zero around 350 nm. Since there is no significant absorption in this region, we attribute this to depolarization resulting from incoherence due to the interaction of multiple beams within the thick sample with the finite bandwidths of the ellipsometer's source and detector.

To determine birefringence, the measured lower right Mueller matrix elements, for a spectral range greater than 400 nm, were first deconvolved from polarization-dependent attenuation. Next, because the order of the retardance is undetermined due to the relative thickness of the sample, there is ambiguity over the true retardance value determined from the deconvolved matrix elements. To address this, a model-based approach in which an extended Cauchy model with four fit parameters was employed to model the birefringence. Fit parameters were generated using the Monte Carlo approach, and the Levenberg-Marquardt algorithm was used to fit the relevant matrix element data to experimental data while minimizing mean squared error between datasets.

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