Spectroscopic Ellipsometry
Room Central Hall - Session EL-ThP

Spectroscopic Ellipsometry Poster Session

EL-ThP-1 Training Neural Networks with Simulated Spectroscopic Ellipsometry Data for Cadmium Telluride Photovoltaic Applications, ***Alexander Bordovalos***, *B. Ramanujam, A. Shan, N. Podraza,* University of Toledo

Ellipsometric spectra can be simulated if the thicknesses and complex index of refraction (*N = n + ik*) spectra are known for the substrate and each layer of the film stack, such as, for example cadmium telluride (CdTe) based thin film solar cells. The ability to generate large data sets of simulated ellipsometric spectra enables the application of machine learning algorithms to spectroscopic ellipsometry data analysis tasks. Based on information learned from the analysis of ellipsometric spectra collected from real CdTe thin films and solar cells, ellipsometric spectra are simulated to assess characterization challenges that could be notably enhanced by machine learning. A promising machine learning task is compositional mapping. A bilayer structure of soda-lime glass / cadmium selenide telluride (CdSe(1-x)Te(x)) where x is one of nine values between 0.037 – 0.81 / cadmium telluride (CdTe) is selected as a proof of concept structure to simulate ellipsometric spectra for training a neural network. Large numbers of data sets are generated for each alloy composition and the thicknesses of the CdSe(1-x)Te(x) and CdTe layers are randomly selected from a common range for photovoltaic applications. A neural network is trained with these data sets to determine which of the nine possible CdSe(1-x)Te(x) compositions was used to simulate the ellipsometry data as well as predict the thickness for the CdSe(1-x)Te(x) and CdTe in the bilayer stack. The neural network determined the correct CdSe(1-x)Te(x) composition 99% of the time on the test set, and 95% of the layer thickness predictions for the CdSe(1-x)Te(x) are within 10% of the ground truth values while 95% of the layer thickness predictions for the CdTe are within 1.2% of the ground truth values. The development of rapid compositional mapping from spectroscopic ellipsometry data could be highly impactful for determining compositional uniformity for thin-film technologies. This approach can be developed further to examine compositional gradient profiles within the film stacks.

EL-ThP-2 Numerical Ellipsometry: Artificial Intelligence for rapid analysis of Indium Tin Oxide films on Silicon, ***Frank Urban***, *D. Barton,* Florida International University

Ellipsometry is a well-known material analytical method widely used to measure thickness and optical properties of thin films and surfaces across a wide range of industrial and research applications including critical dimensions in chipmaking.The method employs the fact that light undergoes a change in polarization state upon reflection from or transmission through a material. The desired properties of the surface structure are related to measurements by the electromagnetic models expressed by Maxwells equations as well as models of material properties. The work here demonstrates the use of Artificial Intelligence (AI) in the form of a multilayer perceptron artificial neural network to apply the electromagnetic model. The reflecting surface examined here is composed of indium tin oxide films (ITO) approximately 400 nm in thickness deposited on silicon substrates. Solutions are provided by 299 artificial neural networks, one per wavelength from 210 nm to 1700 nm across which ITO exhibits transparent as well as absorbing characteristics. Thus, it serves as a proxy for a wide range of other materials. To train the network, simulated measurements are computed at two thicknesses which differ randomly by 1 to 6 nm and at three different incidence angles, 55°, 65°, and 75°. Following training, results are obtained in less than one second on a conventional desktop computer.

EL-ThP-3 Accurate Determination of Critical-Point Parameters in Spectra, *L. Le,* Vietnam Academy of Science and Technology, Viet Nam*; Y. Kim,* Kyung Hee University, Republic of Korea*;* ***David Aspnes***, North Carolina State University

The determination of the locations of critical points of overlapping features in spectra, optical and otherwise, continues to be a challenge even in the absence of complications due to baseline effects and noise.Recent progress in the use of nonlinear (maximum-entropy) methods to eliminate the noise and apodization artifacts characteristic of linear filters, and to detect weak singularities that otherwise would be overlooked, has highlighted the importance of working directly with low-order Fourier coefficients, where information is separated from baseline effects and noise.Here, we report the results of a systematic investigation of critical-point determination in both direct and reciprocal space, with emphasis not only on accuracy but also on uncertainty, using multiple averages of spectra with added noise.Reciprocal-space analysis can be viewed as the logical limit of classic derivative methods of extracting these parameters, which draw conclusions from a relatively narrow range of information-containing coefficients.

EL-ThP-4 Optical Analysis of Ferroelectric PLZT Films Using Spectroscopic Ellipsometry, *S. Kotru,* ***Sneha Kothapally***, The University of Alabama*; J. Hilfiker,* J. A. Woollam Co., Inc.

Spectroscopic ellipsometry was utilized to study the optical properties of ferroelectric lead lanthanum zirconate titanate (PLZT) films. These films were deposited on platinized silicon [Si(100)/ SiO_2/TiO_2/Pt(111)] substrates using the chemical solution deposition method. Films were annealed at two different temperatures (650 and 750 °C) using rapid thermal annealing. Shimadzu UV-1800 UV-VIS spectrophotometer with a resolution of 1 nm was used to measure the reflectance data in the spectral range of 300–1000 nm with a step size of 1 nm. The bandgap values were determined from the reflectance spectra using appropriate equations. A J.A. Woollam RC2 small spot spectroscopic ellipsometer was used to obtain the change in amplitude (Ψ) and phase (Δ) of polarized light upon reflection from the film surface. The spectra were recorded in the wavelength range of 210–1500 nm at an incident angle of 65°. Refractive index (*n*) and extinction coefficient (*k*) were obtained by fitting the spectra (Ψ, Δ) with the appropriate models. No significant changes were observed in the optical constants of PLZT films annealed at 650 and 750 °C. The optical transparency and the strong absorption in the ultraviolet (UV) region of PLZT films make them an attractive material for optoelectronic and UV sensing applications.

EL-ThP-6 Spectrally Resolved Absorption Based Kuhn's Dissymmetry Factor from Mueller Matrix Polarimetry, ***Ufuk Kilic***, University of Nebraska-Lincoln*; A. Ruder, M. Hilfiker,* Onto Innovation*; S. Wimer,* University of Nebraska Lincoln*; E. Schubert, M. Schubert,* University of Nebraska-Lincoln

Chirality or handedness is one of the most intriguing material properties of an object which cannot be made superimposable on its mirror image [1]. Within the last few decades, this symmetry breaking phenomenon has attracted great attention due to its application in various subdisciplines of physics, chemistry and biology [2-4]. The optical manifestation of chirality known as circular dichroism (CD) which is the difference between the absorbance (A) of left circularly of polarized (LCP) light from the right circularly polarized (RCP) light. Recently, Kuhn's dissymmetry factor, so-called g-factor (given as g-factor=2CD/(A_{LCP}+A_{RCP})) is employed as a metric to quantify and compare the chiroptical ability of various systems: nanostructures, molecules, and thin films independent from their fabrication and characterization methods [5]. In this study, we provide a route to reach out the Kuhn's dissymmetry factor in terms of Mueller matrix elements for accurate evaluation and investigation of the chiroptical response of nanostructured thin film samples fabricated via glancing angle deposition technique [6-7]. Therefore, due to the semi-transparent nature of such fabricated structures, it is necessary to reach out both reflectivity and transmissivity properties. Hence, in this study, we present and discuss full road map of obtaining the spectral evolution of Kuhn's dissymmetry factor that utilizes a combinatorial reflection and transmission mode generalized spectroscopic ellipsometry in Mueller matrix configuration. Our method offers the differentiation of circular dichroism information from the other optical anisotropy types which paves the way through a universal and robust method for direct extraction of chirality.

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EL-ThP-7 The Optical Constants of Calcium Fluoride from 0.03 – 9 eV, ***Jaden R. Love***, *C. Armenta,* New Mexico State University*; M. Stokey, M. Schubert,* University of Nebraska - Lincoln*; S. Zollner,* New Mexico State University

In this presentation we describe the optical properties of calcium fluoride (CaF_2), an insulating material for which most optical studies were conducted in the 1960's and are discussed in [1]. Our goal is to reexamine the optical constants of CaF_2 (111) and (100) MTI manufactured substrates in the range 0 – 9 eV using modern ellipsometry equipment and analysis techniques. From these early studies CaF_2 is known to have an ultrawide bandgap of 12 eV, a large exciton binding energy of 1 eV, and a wide transparency range from 125 meV – 10 eV. The large range of transparency makes CaF_2 a suitable material for use in optical components such as those found in infrared detectors and telescopes.

CaF_2 crystalizes in the FCC fluorite structure within the space group Fm-3m and has a lattice constant of 5.4626 Å. Ca 2^+ atoms are in the Wyckoff (4a) position at the origin. F^- atoms are at the (8c) positions (¼, ¼, ¼) and (¼, ¼, ¾). CaF_2 has a three-fold degenerate Raman-active T_{2g} mode and a three-fold degenerate infrared active T_{2u} mode. The T_{2u} mode splits into a transverse optical (TO) doublet and a longitudinal optical (LO) singlet that were observed using infrared ellipsometry and modeled with a Lorentzian. The TO and LO energies are 261 and 477 cm^{-1} , respectively, with an amplitude A = 4.1, a broadening of 4 cm^{-1} , and a high-frequency dielectric constant of 1.98(1). There is a dip in the reststrahlen band formed by two phonon absorption that was modeled using an anharmonically broadened Lorentzian.

Data for the visible and near ultraviolet was obtained using an RC2 ellipsometer and VUV-SE at the University of Nebraska - Lincoln. The data sets were merged to form a continuous spectrum over the range from 0 – 9 eV. In this region the data shows normal dispersion that is modeled using a Tauc-Lorentz oscillator at 7.24 eV and a pole at 9.24 eV. The pseudo-dielectric function $\langle\varepsilon_2\rangle$ is negative above 3 eV indicating the presence of a surface layer with larger refractive index than that of CaF_2. In the region between 7 – 9 eV there is a small peak in $\langle\varepsilon_2\rangle$ modeled by a Gaussian at 7.6 eV with an amplitude A = 0.05. A Cauchy layer was added above the bulk CaF_2 substrate to improve the fit. We determined that the surface layer present on the samples has a thickness of 15 Å.

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EL-ThP-8 Metrology of Ultrathin Iron Catalyst Films by Spectroscopic Ellipsometry, ***Nicholas Allen***, *R. Vanfleet, M. Linford, D. Allred, R. Davis,* Brigham Young University

Vertically aligned carbon nanotube (VACNT) forest growth is a chemical vapor deposition process that uses a thin-film iron catalyst on an alumina support. Iron catalyst thickness for VACNT growth is typically from ~1-10 nm and thickness strongly affects forest morphology. Consequently, characterization of iron thin films could improve process control of VACNT growth. In this study, we explored the use of spectroscopic ellipsometry (SE) to measure these iron thin films because the technique is rapid, highly sensitive, and non-destructive. SE does have challenges, however, as it is difficult to break the correlation in the analysis between the optical constants and thickness of ultra-thin films. The partial oxidization and the absorptive nature of the iron/iron oxide films adds further difficulty. We performed a multi-sample analysis of thermally evaporated iron films with target thicknesses of 1, 2, 4, 7, and 14 nm. To improve sensitivity, we used contrast enhancement by incorporating a 350 nm silicon oxide layer under the iron film and alumina support. We used a consecutive layers approach, collecting SE data and fitting the model for each film before depositing the next. We found high sensitivity to iron thickness with SE, with reproducible thickness results. We modeled the iron/iron oxide film as a composite with an effective medium approximation layer. Our SE model fits the data well with a relatively low mean squared error. We explored the sensitivity of iron/iron oxide thickness results to errors in the alumina thickness while using the consecutive layers approach, which explained most of the variance we found in measured iron thickness.

EL-ThP-9 IR Ellipsometry on Thermally Oxidized Germanium (100), *D. Ortega,* ***Danissa Ortega***, *A. Moses, C. Armenta, J. Love, S. Yadav, S. Zollner,* New Mexico State University

The use of germanium as a semiconductor has been heavily studied but further details about its thermal oxidation, more specifically: its growth methods and process parameters, can show its promise for widespread optoelectronic applications. By performing a Deal-Grove thermal oxidation on bulk Ge, its infrared (combined with ultra-violet) dielectric function can be determined by utilizing J.A. Woollam Vertical Angle Spectroscopic Ellipsometers (VASE) through ellipsometric angles ψ and Δ.

The cleaved 5x10 mm samples were first ultrasonically cleaned in deionized water at room temperature and dried with nitrogen to achieve a native oxide layer of ~1 nm. The samples were then rapidly thermally annealed in ultrapure oxygen at temperatures ranging from 525-575°C in 40 psi pressure for up to 2 hours, reaching thermal oxide layers as high as 35 nm. Spectroscopic ellipsometry measurements were taken using the IR-VASE and UV-VASE to achieve its dielectric function of ψ and Δ in the photon energy range of 0.05-6 eV at room temperature. IR-VASE and UV-VASE measurements were taken at incidence angles from 50-80° which revealed excitations at photon energies ranging 0.09-0.14 eV. The dielectric function was characterized using a two-layer model: the Ge substrate, then the GeO_2 oxide. In the UV range, a Tauc-Lorentz model was utilized, which characterized the fit parameters in the IR range. In the IR range, a Gaussian model fit with peak energy at 0.015 presented a lower MSE than if it were fit with a Tauc-Lorentz or two Gaussians. The modelling will continue to be improved with further growth of the thermal oxide layer at longer annealing times.

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