Spectroscopic Ellipsometry Technical Group
Room Oregon Ballroom 203-204 - Session EL-TuP
Spectroscopic Ellipsometry Poster Session

EL-TuP-1 Dielectric Function of Tantalum Nitride Formed by Atomic Layer Deposition on 300 mm Wafers*, Aaron Lopez Gonzalez*, *Y. Hettige, J. Love, S. Zollner,* New Mexico State University*; E. Bhatia, T. Vo, S. Papa Rao,* NY CREATES

In this undergraduate student poster, we describe the dielectric function of atomic layer deposition (ALD) tantalum nitride (TaN) from 0.03 eV to 6.6 eV determined from spectroscopic ellipsometry.

First, thermal oxides with about 50 nm thickness were grown on B-doped 10 Ωcm Si (100) 300 mm diameter wafers. Tantalum nitride layers with 12 nm and 25 nm thickness were then formed by atomic layer deposition using 300 mm process tools. The TaN layer thicknesses were confirmed by x-ray reflectance (XRR). The TaN surface roughness (also derived from XRR) was on the order of 0.5 nm. On a vertical J.A. Woollam variable angle of incidence rotating-analyzer ellipsometer (V-VASE), the ellipsometric angles ψand Δ were acquired at room temperature at incidence angles from 50° to 80° and photon energies from 0.5 to 6.6 eV with 0.02 eV steps. We used a Berek wave plate compensator and measured with both positive and negative polarizer angles to improve accuracy. We selected a broad range of incidence angles, because the Brewster angle of SiO_2 (55°) is much smaller than that of Si (75°). We also acquired the infrared ellipsometric spectra at the same angles of incidence from 0.03 to 0.70 eV with 8 cm^{-1} resolution on a J.A. Woollam Fourier-transform infrared ellipsometer.

We first developed an ellipsometry model for the optical constants of the thermal oxide, using three Gaussian oscillators at 56, 132, and 146 meV in the infrared spectral region to describe the silicon-oxygen vibrations and a pole at 11 eV (fixed) with variable amplitude to model the visible and ultraviolet dispersion. The TaN layers were described with a Tauc-Lorentz oscillator centered at 3.2 eV with a band gap at 1.7 eV, one UV pole, and one Gaussian in the UV. The fit could be improved with an infrared Gaussian between 0.7 and 1.1 eV, but this peak could be an artifact arising from the uncertainty of the precise layer thicknesses. Across wafer uniformity of the band gap was determined for both thicknesses by performing spectroscopic ellipsometry on coupons from the wafer center, mid radius, and wafer edge. We will perform ellipsometry measurements at low temperatures to investigate the temperature dependence of the optical constants and oscillators.

EL-TuP-2 A Generalized Maximum-Entropy Approach for Eliminating Apodization and Associated Errors in Noise Reduction*, L. V. Le,* Institute of Materials Science, Vietnam Academy of Science and Technology, Viet Nam*; Y. Kim,* Department of Physics, Kyung Hee University, Republic of Korea*; D. Aspnes,* North Carolina State University

In linear filtering, apodization requires compromises to be made among noise leakage, information loss, and Gibbs oscillations (ringing). This problem, inherent in linear filtering, is avoided with the corrected maximum-entropy (CME) procedure. In CME, apodization and associated errors are eliminated by projecting trends established by low-order coefficients into the white-noise region in a model-independent, most-probable way. However, CME cannot be applied to structures that contain an appreciable dispersion-curve component. Capitalizing on Hilbert transforms, we develop a generalized maximum-entropy (GME) approach that can be applied to any lineshape, thereby allowing white noise to be eliminated completely with no deleterious side effects. Endpoint-discontinuity removal and a Hilbert transform can reversibly convert any segment consisting of a Lorentz/dispersion combination into an absorption spectrum, thus allowing any spectrum to be processed by CME. As an added benefit, Hilbert transforms are exact Kramers-Kronig (KK) transforms of these segments, providing new opportunities for analysis in spectroscopy.

EL-TuP-3 Intelligent Linear Filters for Noise Reduction in Spectroscopy*, Young Dong Kim,* Kyung Hee University, Republic of Korea*; L. Le,* Vietnam Academy of Science and Technology, Viet Nam*; D. Aspnes,* North Carolina State University

A linear filter must strike a balance among reducing noise, preserving lineshapes, and minimizing or eliminating ringing. While nonlinear methods offer superior performance, direct- (spectral-) space (DS) convolution is convenient and may be sufficient in many applications. However, optimization requires reciprocal- (Fourier-) space (RS) considerations. This follows because information appears as point-to-point correlations and noise as point-to-point fluctuations, thereby concentrating information and noise in low- and high-order Fourier coefficients, respectively. For optimum performance, the transfer function of any filter must be consistent with the Fourier transform of the spectrum.

Using Parseval's Theorem, we project typical DS performance measures such as mean-square error (MSE) into RS. The resulting expressions are simpler and more informative than their DS counterparts, providing quantitative insight not only into the effectiveness of different linear filters, but also how they can be improved. Surprisingly, the rectangular ("ideal" or "brick wall") filter is found to be nearly optimal, a consequence of its complete elimination of distortion in low-order coefficients. When ringing is taken into account, the best practical filter is the Gauss-Hermite. Capitalizing on the information provided by these calculations, we develop a version that is demonstrably superior to both brick-wall and Gauss-Hermite filters.

EL-TuP-4 Temperature Dependence of the Fine Structure of the NiO Critical Points*, Yoshitha Hettige,* *C. Armenta, J. Love, S. Zollner,* New Mexico State University*; M. Veis,* Charles University, Prague, Czech Republic

Nickel oxide (NiO) is a cubic charge-transfer insulator. Its valence band consists of Ni 3d and O 2p states. The Ni 3d states split into t_{2g} and an e_g bands. The valence band maximum is a hybridized mixture of O 2p and Ni e_g states. The excited e_g^* band is about 4 ev above the eg band. Optical interband transitions from e_g into e_g^* give rise to a strong absorption peak near 4 eV known as the charge transfer gap. The location of the Ni 4s band is not clear.

In addition to the strong charge transfer gap at 4 eV, there are two other features in the optical spectra of NiO. (1) There is a small amount of absorption between 1 and 4 eV (similar to the indirect absorption of Si) in the pseudodielectric function, which cannot be explained with surface roughness. It is possible that this absorption is due to defects, such as excess oxygen. (2) There are several weak peaks between 1.5 and 4.0 eV. They might be due to interatomic transitions between the Ni 3d orbitals. The temperature dependence of these weak peaks (which we call fine structure) is the topic of this abstract.

In this presentation, we will discuss the temperature dependence of the smaller peaks in these spectra and attribute them to features in the band structure of NiO.

EL-TuP-5 Characterization of Hybrid Organic-Inorganic Perovskite Semiconductors and Solar Cells*, Bailey Frye,* *E. Miller, N. Podraza,* University of Toledo

Hybrid organic-inorganic lead-halide based perovskite semiconductors (ABX_3) are absorber layers in high efficiency single junction and tandem thin film solar cells. The ability to modify the bandgap energies over a wide range is required for these applications, with typical components consisting of an organic molecule A-cation such as methylammonium (MA) or formamidinium (FA), metal B-cation such as Pb or Sn, and a halogen X-anion such as I or Br. Spectroscopic ellipsometry is the ideal characterization technique for determining the complex dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) spectra and thickness of these perovskites as thin films or within solar cell device structures. Various oscillator models have been used to describe ε for these direct-gap, polycrystalline semiconductors. Many models may generate an approximate line shape for ε, but unfortunately lack physically meaningful parameters, are not Kramers-Kronig (KK) consistent — and therefore not physically realistic, or require numerical integration of the KK-integral that is often prohibitively time consuming. A KK-consistent parametric model that uses excitonic critical point parabolic band (CPPB) oscillators and an Urbach tail is presented in this work. CPPBs represent the band-to-band transitions of a semiconductor, including the bandgap, while the Urbach tail describes subgap absorption features. $\varepsilon_2$is described by a series of CPPB oscillators with an Urbach tail and then $\varepsilon_1$is determined from the analytic solution to the KK-integral of ε_2. This parametric model is thus KK-consistent with physically meaningful parameters relevant to direct gap crystalline semiconductors and is shown to model experimental ellipsometric spectra and describe the line shape of ε accurately and quicklyfor various compositions of hybrid organic-inorganic lead-based perovskite semiconductors. This model may be of great use for analyses of perovskite semiconductors that require many data sets, such as real time spectroscopic ellipsometry and ellipsometric spatial mapping. Applications of this CPPB and Urbach tail model to the analysis of ε for

polycrystalline $(FASnI_3)_{1-x}(MAPbI_3)_x$, spatial mapping of $FA_{0.8}Cs_{0.2}Pb(I_{0.65}Br_{0.35})_3$ and $FA_{0.8}Cs_{0.2}Pb(I_{0.6}Br_{0.4})_3$ films including those in the partial and full device structures, and through-the-glass ellipsometry of full solar cells containing perovskite absorber layers are presented in this work.

EL-TuP-6 Many-Body Effects in the Mid-Infrared Dielectric Function of InSb from 80 to 800 K*, M. Rivero Arias, C. Armenta,* New Mexico State University*; C. Emminger,* Leipzig University, Germany*; C. Zamarripa,* New Mexico State University*; N. Samarasingha,* Nova Measuring Instruments*; J. Love, S. Yadav, **Stefan Zollner**,* New Mexico State University

We describe measurements of the mid-infrared dielectric function of bulk InSb near the direct band gap using Fourier-transform infrared spectroscopic ellipsometry from 80 to 800 K in an ultra-high vacuum cryostat. Indium antimonide is the zinc blende compound semiconductor with the smallest direct band gap (E0=0.18 eV at 300 K) due to its heavy elements and the large resulting spin-orbit splitting and Darwin shifts. The band gap is extracted from the dielectric function by fitting with a parametric oscillator model. It decreases from 80 to 450 K following a Bose-Einstein model, then remains constant up to 550 K, and increases again at the highest temperatures. This is explained with a thermal Burstein-Moss shift: The onset of optical absorption increases as electron-hole pairs are thermally excited at the highest temperatures. The intrinsic carrier concentration determined from the Drude tail in the ellipsometry spectra agrees qualitatively with temperature-dependent Hall experiments and calculations based on degenerate Fermi-Dirac statistics.

EL-TuP-8 Film-Side Versus Through-the-Glass Ellipsometry Measurements of Wide Band Gap Perovskites*, **Emily Amonette**, K. Dolia, B. Frye, Y. Yan, Z. Song, N. Podraza,* University of Toledo

Wide band gap $FA_{0.8}Cs_{0.2}Pb(I_{1-x}Br_x)_3$ (x = 0.3, 0.35, 0.4) perovskite thin films are examined via spectroscopic ellipsometry in both the film-side mapping configuration and as part of complete superstrate photovoltaic (PV) devices. Complex dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) spectra of the perovskite and all layer thicknesses are determined for all measured samples. Film-side measurements are more commonly performed, and it is often assumed that the resulting ε spectra represent a layer in a complete device, but this work examines variations in perovskite ε and associated characteristics such as the band gap and Urbach energies that may only be apparent when considering data from a complete PV device taken in the through-the-glass configuration. Measurements of partial device-like structures consisting of glass superstrate / indium tin oxide / hole transport layer / perovskite reveal spatial variations in band gap energies ranging from 1.77 to >1.80 eV in the case of $FA_{0.8}Cs_{0.2}Pb(I_{0.6}Br_{0.4})_3$ as well as variations in Urbach energies, while those of complete PV devices consisting of the same structure and perovskite composition but completed with the electron transport layer and metal back contact exhibit less spatial variation, where band gap energies vary only between 1.75 to 1.77 eV. This behavior indicates that atmospheric exposure amplifies perovskite material spatial uniformity. Optical property and thickness information from through-the-glass ellipsometry is used to simulate external quantum efficiency (EQE) spectra, and by comparing these simulations to experimental EQE, information about both optical and electronic loss in PV is obtained.These data sets comprised of many similar but slightly different samples and measurement configurations are used to develop methods for streamlining the analyses, such as considering which parameters may be kept common to multiple samples and how to deal with outliers resulting in substantially different optical properties and PV device performance. These patterns in parameter values may also predict success in accurately calculating PV device performance parameters from EQE simulations as well as develop strategies for analyzing large amounts of data sets.

EL-TuP-9 Determination of the Optical Constants and Thickness of Ultrathin Thermally Evaporated Iron Catalyst Films Using Spectroscopic Ellipsometry*, **Nicholas Allen**, M. Linford, R. Vanfleet, R. Davis,* Brigham Young University

Vertically aligned carbon nanotube (VACNT) forest growth is a catalytic 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. Transmission electron microscopy has been used to directly measure the thicknesses of thin iron/iron oxide films but is destructive and not easily used for routine process monitoring. Atomic force microscopy has also been used but requires the creation of an abrupt step edge in the film. Here we describe the use of spectroscopic ellipsometry for characterization of these very thin iron films. However, in this thickness range, the optical constants and thickness are not easily separated. The absorptive nature of the iron/iron oxide films adds further difficulty. In this study, a multi-sample ellipsometry analysis was performed using iron films of various thicknesses to obtain the optical constants of thermally evaporated iron. We also explored contrast enhancement by incorporating a silicon dioxide layer under the film being analyzed to enhance sensitivity to the optical constants.

EL-TuP-10 Elevated Temperature Model Dielectric Function of InAs Determined by Spectroscopic Ellipsometry*, **Preston Sorensen**, U. Kilic, R. Korlacki, M. Schubert,* University of Nebraska - Lincoln

We report a model dielectric function approach to determine and predict the elevated temperature (30-250°C) dielectric function of InAs across the spectral range of the near infrared to deep ultraviolet (0.73eV to 5.0eV). InAs is a III-V zincblende structure semiconductor with low-energy direct bandgap of 0.355eV and is of interest in long wavelength optoelectronic devices [1,3,4]. Determining accurately the thermal evolution of its optical properties, such as its complex index of refraction, bandgap energy, and band to band transitions permits for improved prediction of its thermal behavior in devices under operation. Also, knowledge of the dielectric function variation with temperature enables model-based analysis of spectroscopic ellipsometry data of InAs-based layer structures. Thermal perturbation of a crystal results in a small increase in the lattice constant of the material, altering the band structure, and therefore its dielectric function [4]. Spectroscopic ellipsometry permits measurement of the dielectric function of InAs. Measurements were taken from 30 ^{o}C to 250 ^{o}C at a single angle of incidence utilizing the temperature-controlled sample compartment of an atomic layer deposition system. The sample was also measured at room temperature at multiple angles of incidence in normal ambient to identify surface over layer effects. All ellipsometry data were modeled using a critical-point model dielectric function approach with implemented temperature dependencies of all the critical point model parameters [2,3]. We find linear evolutions of all critical-point model parameters versus temperature for the investigated temperature range. The obtained model parameters permit accurate prediction of the dielectric function of InAs at any temperature in the investigated range. Our result can be useful for model-based quantitative analysis of in-situ ellipsometry data obtained during atomic layer deposition growth of layer structures on InAs substrates.

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EL-TuP-11 Numerical Ellipsometry: Artificial Intelligence for Real-Time, *in Situ* Absorbing Film Process Control*, **Frank Urban**,* Florida International University*; D. Barton,* Florida International University Retired

Ellipsometry is a material analytical method in which the desired parameters, for example film thickness and index of refraction, are related to the instrument measurements through Maxwell's equations, light wavelength, and measurement geometry. Consequently, obtaining the desired parameters has required solving the model equations using a wide variety of methods. A commonly used method is least squares curve fitting, frequently the Levenberg-Marquardt method. This numerical method depends upon not only the model but also the initial estimates of solution, the possible interference of local minima, and the algorithm stopping conditions. Being iterative, it also can take significant time. The work here demonstrates the use of Artificial Intelligence in the form of a multilayer perceptron artificial neural network to avoid these problems and find solutions in the microsecond time scale. This non-iterative, stable, and fast performance lends itself to real-time, *in situ* monitoring of thin film growth. Examples for thin (up to 30 nm) films will be given using a multilayer perceptron configuration consisting of 4 input and 4 output neurons with two hidden layers of up to 20 neurons each. Solutions are performed at each wavelength independently and do not rely on fitting functions for optical properties.

EL-TuP-12 Massive Data Collection With A Pupil Plane Imaging Polarized White Light Interferometer, ***Alexander Boosalis,*** *Y. Wang,* Onto Innovation; *P. Vagos,* Onto Innovation, France; *Y. Liu,* Onto Innovation, Singapore; *G. Antonelli, N. Smith,* Onto Innovation

We present novel instrumentation capable of measuring the Jones matrix response of a sample across a large range of incident angles (0-55 degrees), sample rotation angles (0-360 degrees), and wavelengths (400-1000 nm) in less than 10 seconds. The result is a massive data set with over 600,000 individual data points. Development of this tool was spurred by the requirements of commercial chip manufacturing to collect and process a large amount data for optical critical dimension (OCD) metrology in the smallest possible time and within a shrinking measurement area. However, this instrument is increasingly applicable to the research community where development of metasurfaces, biaxial thin films, and other complex nanostructures requires measurement over a range azimuth angles to properly characterize. The instrument also has a small measurement spot size – less than 10 um in diameter – which is useful for both OCD metrology and prototype research nanostructures which tend to be hard to produce over large areas. We will demonstrate a prototype tool measuring an industry standard calibration scatterometry target with a 10um box size.

The white light interferometer is in a Linnik configuration with high numerical aperture objectives. By imaging the back focal plane of the sample objective to a camera we can collect a white light interferogram at every pixel that contains both reflection amplitude and phase information over a wide array of incidence angles. In this configuration the instrument lies somewhere between the capabilities of a polarized reflectometer and a rotating analyzer ellipsometer at each individual angle of measurement, with sensitivity to the entire Jones matrix but not the ability to measure the Jones elements specifically. We will show that rotating the system polarizer allows determination of the individual Jones matrix elements.

EL-TuP-13 Fast Spectroscopic Mueller Matrix Ellipsometry in the THz Range, ***Alexander Ruder,*** University of Nebraska - Lincoln; *S. Richter,* Lund University, Sweden; *P. Kuhne,* Linkoping University, Sweden; *V. Rindert,* Lund University, Sweden; *V. Stanishev,* Linkoping University, Sweden; *R. Korlacki, J. Olander,* University of Nebraska - Lincoln; *V. Darakchieva,* Lund University, Sweden; *M. Schubert,* University of Nebraska - Lincoln

We demonstrate a spectroscopic Mueller matrix ellipsometer in the THz wavelength range using rotating anisotropic optical components for polarization state generation and analysis. A solid state source and detector allow for time division multiplexing of individual wavelengths at kHz rates. Synchronous modulation of the source wavelength, polarization state generator, and polarization state analyzer allows for rapid acquisition of 4x4 Mueller matrix spectra. Calibration procedures and initial results for isotropic and anisotropic samples are discussed.

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