Monday Morning, November 6, 2023

Spectroscopic Ellipsometry Technical Group
Room C124 - Session EL1-MoM

Big Data, AI and Analytical Methods

Moderators: David Aspnes, North Carolina State University, **Tino Hofmann**, University of North Carolina at Charlotte

8:20am **EL1-MoM-1 Ellipsometry Analysis Overview: Things We Can't Ignore***, **Nikolas Podraza**, A. Bordovalos,* University of Toledo*; P. Dulal, N. Jayswal, M. Mainali, E. Miller, B. Shrestha, M. Tumusange, R. Collins, A. Shan,* University of Toledo, United States Minor Outlying Islands (the) **INVITED**

Most spectroscopic ellipsometry measurements are relatively straightforward to make (but still must be done with care), however the analyses may not be straightforward even for seemingly simple samples.Appropriate and justifiable structural and optical property models must be developed to obtain meaningful information from measured ellipsometric spectra.However, even after substantial time spent analyzing data all of us in the field ask:"Is this the correct model?"More complicated measurement configurations and simultaneous analysis of multiple sets of spectra can either help answer that question or make the situation even more challenging and uncertain.A follow up question also becomes "When do I stop?"Many of us have also spent long amounts of time (sometimes far more time than we should in retrospect) trying to describe small, nuanced features in our measured spectra that we simply can't ignore.To answer those questions, there are also things we can't ignore in the analyses of ellipsometric spectra including if the structural model makes sense; if the complex optical properties obtained are Kramers-Kronig consistent and appropriate for the type of material and spectral range measured; the extent of surface or interfacial layer effects and our ability to describe them meaningfully; and of course the parameters of interest to be extracted from our models, quality of fit, confidence limits, and correlation matrices.These considerations will be discussed for metallic, semiconducting, and dielectric thin film and bulk materials characterized by spectroscopic ellipsometry spanning the ultraviolet (UV) to terahertz (THz) range.This will include strategies for analyzing thin films with unknown optical properties, samples with complicated structures (and knowing when to stop), mapping spectroscopic ellipsometry data, and in situ real time spectroscopic ellipsometry data.Most examples we will discuss are materials used in thin film polycrystalline solar cells based on hybrid organic inorganic lead halide based perovskites, cadmium telluride, and copper indium gallium diselenide absorbers as well as spectroscopic ellipsometry characterization of complete, functional solar cells.

9:00am **EL1-MoM-3 Noise Reduction Using Linear and Nonlinear Filtering***, **Long V. Le**,* Institute of Materials Science, Vietnam Academy of Science and Technology, Viet Nam **INVITED**

If lineshape distortion and loss of information are not factors, linear low-pass filters are very effective at eliminating noise from spectra. However, achieving the balance among lost information, leaked noise, and Gibbs oscillations (ringing) can be difficult. Many linear filters are available that operate with direct-(spectral) space (DS) convolution. This approach is convenient, and endpoint discontinuities in value or slope have only local effects. However, intelligent linear filtering requires assessments in reciprocal-(Fourier) space (RS), capitalizing on the separation of information and noise into low- and high-index Fourier coefficients, respectively. Comparing the information content of the data to the RS transfer function of the filter is necessary if filtering is to be performed intelligently.

We recently quantified the tradeoff between reducing noise and preserving information by capitalizing on Parseval's Theorem to cast two DS measures of performance, mean-square error (MSE) and noise, into RS. This provides quantitative insight not only into the effectiveness of the various linear filters but also information on how they can be improved. The best practical linear filter was found to be the Gauss-Hermite filter introduced about 20 years ago by Hofmann and co-workers.

Nonlinear filters have an interesting history, which is reviewed briefly. Originally designed to "whiten" (sharpen) structure in spectra, a recent solution of Burg's equations allows the trend established by low-index Fourier coefficients to be extrapolated into the white-noise region in a model-independent way. This corrected-maximum-entropy (CME) filter achieves all 3 goals: information is left intact, noise is eliminated, and by eliminating apodization, ringing is also eliminated. Recent progress includes adapting the theory to filter general lineshapes. By introducing an enhancement factor in the ME equations, weak features can be discovered and structures enhanced without the complications inherent in Burg's original result. Examples will be provided throughout, along with MATLAB programs that perform the processes discussed.

9:40am **EL1-MoM-5 Numerical Ellipsometry: Artificial Intelligence Methods for Solving Ellipsometer Data***, **Frank Urban**, D. Barton,* Florida International University

Ellipsometry is a material analytical method which works by measuring the change in polarization state of light reflecting from or transmitting through the material of interest.Desired parameters, such as thin film thickness and optical properties, are related by mathematical models to the measurements themselves. In the beginning those parameters were obtained by lookup using a printed table provided along with a commercial ellipsometer.This was followed by solution methods using a calculator and this evolved to the personal computer based programs that are in use today.Because a single ellipsometer measurement provides two real numbers, typically Ψ and Δ, it can provide for determination of only two unknowns associated with the reflecting surface regardless of whether other measurement modes are employed such as Mueller matrix forms.As a consequence it usually became necessary to make use of more than a single measurement at a single wavelength to obtain more than two parameters.Two of the ways forward are to take multiple measurements at each wavelength of interest to obtain data sufficiency and the other way is to take spectroscopic measurements with the aim of solving for optical constants as represented as various functions (fitting functions) of wavelength.For the spectroscopic approach the match to the Maxwell equations and to the selected "fitting functions" by which the number of unknowns is reduced hugely by the small number typically three or four per fitting function.Thus data sufficiency is achieved at the cost of requiring good selections of fitting functions which might not be unique.We have found, following earlier work, that current Artificial Intelligence methods in the form of Deep Learning or Artificial Neural Networks offers a new way to obtain solutions or at least to provide very accurate initial estimates from which numerical method solutions can reliably and accurately be determined.The work presented here both covers a two measurement method AI network at single wavelengths and spectroscopic measurements (a thousand or more) using fitting functions.Accuracy, speed, and ease of use will be demonstrated.

10:00am **EL1-MoM-6 Modeling Many-body Effects in Ge Using Pump-Probe Time-Resolved Spectroscopic Ellipsometry***, **Carlos A. Armenta**,* New Mexico State University*; M. Zahradnik, M. Rebarz,* ELI Beamlines Facility, The Extreme Light Infrastructure ERIC, Czechia*; S. Espinoza,* ELI Beamlines Facility, The Extreme Light Infrastructure ERIC*; S. Vazquez-Miranda,* ELI Beamlines Facility, The Extreme Light Infrastructure ERIC, Czechia*; J. Andreasson,* ELI Beamlines Facility, The Extreme Light Infrastructure ERIC*; S. Zollner,* New Mexico State University

We analyze the transient dielectric function (TDF) of Ge at very high electron-hole pair densities via time-resolved spectroscopic ellipsometry. Through a pump-probe technique, the bulk Ge is photoexcited up to densities of around $\sim 3\times10^{21}$ cm^{-3}. We specifically focus on the E_1 and $E_1+\Delta_1$ critical points and how their parameters such as energy and broadening change as a function of delay time.

Our analysis aims to model the TDF of Ge and describe its behavior at different carrier concentrations. In particular, it addresses phase-filling singularities that are usually difficult to study in implanted and annealed samples due to defects. High-power laser induced carriers can achieve density levels on undoped samples that are ideal for the study of many-body phenomena. The model also addresses other effects taking place during the excitation and relaxation of electrons, such as excitonic screening and acoustic phonon oscillations produced by the transferring of energy to the lattice.

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