

# Thursday Evening Poster Sessions

## Spectroscopic Ellipsometry Focus Topic

Room: Hall 3 - Session EL-ThP

## Spectroscopic Ellipsometry Poster Session

### EL-ThP2 Phonon Dispersion and Electronic Band Structure of NiO,

*Stefan Zollner, A. Ghosh, T. Willett-Gies, New Mexico State University, C. Nelson, University of New Mexico, L. Abdallah, New Mexico State University*

The phonon dispersion and the electronic band structure of bulk NiO were investigated at 300 K using spectroscopic ellipsometry from the mid-infrared (0.03 eV) to the near-ultraviolet (6.5 eV). Since NiO crystallizes in the rocksalt structure, we find a single transverse-optical (TO) phonon at 49 meV with a broadening of 2 meV. There is no evidence of mode-splitting (due to antiferromagnetic ordering, within the broadening of this phonon of 2 meV) or zone folding (due to the doubling of the unit cell). Instead, we find a modification of the reststrahlen band due to TA+TO two-phonon absorption occurring between the TO and LO phonon energies, similar to LiF. Using transmission and ellipsometry measurements, we clearly establish that the lowest direct band gap of NiO occurs at 0.85 eV at room temperature. The valence band maximum (VBM) of NiO is made up of O (2p) states and the lower Hubbard band of the Ni (3d) states. Direct interband transitions at 0.85 eV are possible from the valence band to the dispersive Ni (4s) conduction band at the  $\Gamma$  point. A strong peak in the absorption at 3.95 eV is attributed to transitions from the valence band to the upper Hubbard band (the charge transfer gap of NiO). A derivative analysis of the ellipsometry spectra also shows weak peaks at intermediate energies (between 1.7 and 3.6 eV), which are attributed to transitions from localized valence band states to the dispersive Ni (4s) band. The charge-transfer gap of NiO shows a temperature dependence very similar to the  $E_g$  gap of Si. The absorption between 1 and 3 eV has a very different behavior, however. The character of the pseudo-dielectric function of NiO changes completely between 700 and 800 K in UHV, where NiO is known to deteriorate due to sublimation. Cooling the sample does not restore the original shape of the dielectric function, but it can be recovered partially by annealing in oxygen.

### EL-ThP3 Tribrid EC-QCMD-GSE Analysis: Surface Topography Effects on the Electrochromic Behavior of Methylene Blue, *Derek Sekora, A.J. Zaitouna, R.Y. Lai, T. Hofmann, M. Schubert, E. Schubert, University of Nebraska - Lincoln*

The optical and electrical properties of flat and highly ordered, 3-dimensional nanostructured thin films change dramatically upon adsorption of self assembled monolayers (SAMs) to the surface. Here, a tribrid technique consisting of electrochemistry (EC), quartz crystal microbalance with dissipation (QCM-D), and generalized spectroscopic ellipsometry (GSE) is introduced which allows for fundamental analysis of simultaneous electrochemical, optical, and mechanical properties. The electrochromic reduction of methylene blue terminated SAMs on flat and slanted columnar thin film Au substrates is investigated as an example.

The electrochemical redox reaction of methylene blue produces a switch between a blue and colorless SAM, which can be ellipsometrically modeled. Furthermore, a combinatorial tribrid analysis of in-situ step-decreased constant potential scans elucidate the effects of varying the quantity of reduced methylene blue molecules on flat and nanostructured surfaces. The EC and GSE results imply that methylene blue molecules attached deep between Au slanted columns are not as readily reduced as a result of capacitive shielding effects at lower cell potentials. The concurrent in-situ QCM-D response indicates no quantifiable mass transfer as expressed by the Sauerbrey analysis. The results demonstrate that the fluidic tribrid technique allows characterization of conformal coatings on highly ordered nanostructured surface topographies during electrochemical surface modifications. Our approach is perfectly suited for applications including DNA sensing procedures, electrochemical surface reactions, and surfactant effects.

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