Spectroscopic Ellipsometry Focus Topic
Room: Hall B - Session EL-ThP

Spectroscopic Ellipsometry Poster Session

EL-ThP2 Electronic and Vibrational Properties of Nickel Oxide using Spectroscopic Ellipsometry, ***C.M. Nelson***, *T. Willett-Gies, L.S. Abdallah, S. Zollner*, New Mexico State University

Nickel oxide (NiO) is an interesting material, because it is a Mott-Hubbard charge-transfer insulator and also displays antiferromagnetic ordering of electron spins [1]. Spectroscopic ellipsometry is able to investigate the electronic structure of NiO (from the visible and UV portions of the spectra) and also its lattice dynamics (using infrared ellipsometry). Our interest in the NiO optical constants is also of a practical nature, to model ellipsometry spectra of bulk Ni and Ni thin films with a native oxide of NiO.

We measured the ellipsometric angles ψ and Δ for single-side polished bulk NiO from 0.8 to 6.5 eV with angles of incidence from 65 to 75° to determine the dielectric function. A dispersion model for the optical constants was built using two Tauc Lorentz oscillators; one with a Lorentz oscillator resonance energy at 3.96 eV and a second one with a much smaller amplitude at 6.40 eV. These peaks are in agreement with reflectance data analyzed using Kramers-Kronig transforms [2]. Our model also included a surface roughness layer with 40 Å thickness. Atomic force microscopy measurements confirmed this layer, showing an RMS roughness of 42.5 Å. We will report accurate dielectric function data for NiO from 0.8 to 6.5 eV.

FTIR ellipsometry was also performed on bulk NiO from 290 to 1000 cm^{-1} to study the lattice vibrations. TO phonons were found at 392 cm^{-1} and 551 cm^{-1}, with the corresponding LO modes at 592 cm^{-1} and 545 cm^{-1}. The weak TO mode at 551 cm^{-1} results from the antiferromagnetic ordering of NiO, which doubles the unit cell and causes zone folding, making a zone-edge TO mode infrared-active. Previous FTIR absorption measurements of NiO [3] did not report the infrared-active zone-edge phonon. Usually, antiferromagnetic ordering is only observed using neutron scattering, not with FTIR optical methods.

[1] G.A. Sawatzky and J.W. Allen, Phys. Rev. Lett. **53**, 2339 (1984).

[2] R.J. Powell and W.E. Spicer, Phys. Rev. B **2**, 2182 (1970).

[3] R. Newman and R.M. Chrenko, Phys. Rev. **114**, 1507 (1959).

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EL-ThP3 Properties of Sm Doped CeO_2 Thin Films Prepared by Liquid Solution Deposition, *K.N. Mitchell, C.A. Rodriguez, T. Willett-Gies, Y. Li,* ***S. Zollner***, New Mexico State University

Cerium(IV) oxide, also known as CeO_2 or ceria, is a transparent (insulating) oxide of the rare earth metal cerium. It is an ionic conductor with applications in fuel cells, as a catalyst, or for photovoltaic water splitting (hydrogen production). Thin films of ceria produced by RF magnetron sputtering on sapphire at 770C have been studied extensively by Arwin's group (S. Guo et al., J. Appl. Phys. 77, 5369, 1995). They found changes in grain size, surface morphology (visible in AFM images), and optical constants varying with the film thickness. By contrast, we report analysis results for relatively thick (300-500 nm) ceria films prepared by liquid solution deposition (dip-coating) followed by annealing. We also investigate the effect of samarium doping (up to 20at.%) of ceria. The rare earth metal samarium usually forms a sesquioxide Sm_2O_3. Therefore, doping ceria with Sm is expected to lead to the formation of oxygen vacancies, which enhances the ionic conductivity of ceria. Our ellipsometry spectra (ellipsometric angles and depolarization) can be described very well in the transparent region (below 3 eV) using a Tauc-Lorentz dispersion model for ceria, if small amounts of surface roughness and thickness non-uniformity across the wafer are taken into account. Once these thickness parameters have been determined for our films, we obtain the optical constants of CeO_2:Sm using a basis spline expansion. We find the typical dispersion expected for an insulator with a direct band gap near 3.7 eV. Samarium doping causes a significant decrease of the refractive index in the transparent region. Most likely, the films with high Sm content are less dense (have more voids, perhaps due a smaller crystallite size) than pure ceria films. An increase in disorder due to Sm doping was also found in x-ray diffraction studies of electrodeposited ceria films (Phok and Bhattacharya, phys. status solidi (a) 203, 3734, 2006). As expected from Kramers-Kronig consistency, we find a significant reduction of the height of the main absorption peak at 4 eV. The direct band gap, however, remains at 3.7 eV, independent of Sm content. There is, however, a significant decrease in the slope of the onset of absorption with increasing Sm content. In addition to ellipsometry results, we will also report AFM, XRD, Raman, and (perhaps) FTIR ellipsometry results for our Sm-doped ceria films.

Authors Index

Bold page numbers indicate the presenter