Spectroscopic Ellipsometry Technical Group
Room C124 - Session EL1+TF-MoA

Thin Films & Novel Materials

Moderators: Mathias Schubert, University of Nebraska - Lincoln, **Megan Stokey**, Milwaukee School of Engineering

1:40pm **EL1+TF-MoA-1 Enhancement of Electron Effective Mass in Semiconductor Materials and 2DEGs Revealed by THz Optical Hall Effect**, ***Nerijus Armakavicius,*** Linköping University, Sweden*; S. Knight,* Linköping University*; P. Kuhne, H. Zhang, R. Carrascon,* Linköping University, Sweden*; S. Richter,* Linköping University, Lund University, Sweden*; V. Stanishev,* Linköping University, Sweden*; M. Schubert,* Linköping University, Sweden, University of Nebraska-Lincoln*; P. Paskov,* Linköping University, Sweden*; V. Darakchieva,* Lund University, Sweden **INVITED**

Progress in semiconductor material technology continues to enable significant advances in nearly all scientific endeavors and lies at the heart of modern information and communication networks. Wide band gap semiconductors, such as GaN and SiC transpire as key materials to address the demands of next-generation quantum technology and green electronics.Understanding transport in semiconductor materials is a prerequisite for their implementation in advanced device architectures with improved functionalities. Electron effective mass is a fundamental material parameter defining the free charge carrier transport but it is very challenging to be directly determined at high temperatures and frequencies relevant for device operation.

With the advent of the optical Hall effect (OHE), which consists of performing generalized spectroscopic ellipsometry at long wavelengths in magnetic field the determination of the electron effective mass tensor at variable temperatures has became possible without the need to invoke any additional electrical measurements [1,2]. The OHE describes the external magnetic field induced anisotropic charge displacement in materials when interacting with electromagnetic waves and allows for the determination of the charge carrier sign, concentration, mobility and effective mass parameters [2].

In this work, we present a comprehensive investigations of the electron effective mass parameters in GaN bulk and epitaxial layers, as well as in two-dimensional electron gas (2DEG) in GaN based high-electron mobility transistor structures [3,4] by THz and MIR OHE [5]. OHE analysis allows to extract the free charge carrier concentration and mobility in the various structures as a function of temperature and the results are found to be in a good agreement with the respective parameters obtained by electrical Hall effect and capacitance-voltage measurements. In addition, the electron effective mass parameter is determined from the OHE at temperatures from 10K to 370K. At low temperatures (< 100 K) an electron effective mass of approximately $0.20m_0$ is obtained in agreement with the well accepted value. Unusual enhancement of the electron effective mass is discovered with increasing temperatures to room temperature and above for both bulk, epitaxial and 2DEG GaN systems. We evaluate and discuss various mechanisms such as band gap nonporabolicity, magnetic field, strain and polaron effects,that could potentially contribute to the observed increase. We propose a frequency-dependentscattering time to be at the origin of the effective mass enhancement. We also discuss possible deviations of the free electron behavior from the classical Drude model and its implications for transport and devices operating at high temperatures (room temperature and above) and frequencies (100 GHz to 1THz).

References

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2:20pm **EL1+TF-MoA-3 In Situ and Real Time Spectroscopic Ellipsometry of Polycrystalline $CuInSe_2$ Co-Evaporation for Narrow Bandgap Photovoltaic Absorbers**, *D. Sapkota,* ***Balaji Ramanujam****, M. Alaani, A. Shan, N. Podraza, R. Collins,* University of Toledo

Deposition processes for narrow bandgap (E_g = 1.02 eV) polycrystalline $CuInSe_2$ (CIS) thin films with intended applications as photovoltaic (PV) absorbers have been developed and studied using various techniques of in situ and real time spectroscopic ellipsometry (SE). Real time SE analyses of two series of sequentially deposited Cu and In_2Se_3 thin films on the same substrates, but at different Cu and In evaporation source temperatures, serves as an accurate source calibration method. This calibration enables co-evaporation of CIS films at independently controllable deposition rates and compositions, the latter characterized by the [Cu]/[In] molar ratio which establishes their p-type character as PV absorbers. In situ SE analyses of the starting crystalline Si substrates provide an accurate substrate temperature calibration, and real time SE of CIS co-evaporation on such substrates provides insights into polycrystalline nucleation and grain coarsening processes. In contrast to earlier studies of hydrogenated amorphous silicon PV absorbers, the highest device quality CIS absorbers are obtained in processes leading to the most extensive increases in the surface roughness layer thickness with bulk layer thickness, characteristic of crystallites of increasing size protruding from the film surface. Real time SE provides the time evolution of the surface roughness layer, bulk layer, and effective thicknesses for the deposited film, where the effective thickness is the volume per planar area of substrate and, thus, includes the surface roughness contribution. The effective thickness is used to evaluate the deposition rate for the desirable situation in which the roughness thickness increases continuously with bulk layer thickness. For substrate temperatures of 500°C and below in CIS co-evaporation, the roughness thickness is relatively stable with increasing bulk layer thickness at values controlled by the initial nucleation. At higher temperatures, in contrast, the surface roughness thickness increases rapidly and continuously with bulk layer thickness, well above that observed in the initial nucleation process. Such grain growth enhancement is also reflected in the following variations in the final film properties with increasing substrate temperature: (i) an increased grain size as determined by the widths of the peaks in the X-ray diffraction pattern, (ii) a reduction in the bandgap critical point broadening parameter from ex situ SE, consistent with an increase in the grain boundary scattering time for excited carriers, (iii) a steeping of the Urbach tail, and (iii) higher performance PV devices for absorbers incorporated into cell structures.

2:40pm **EL1+TF-MoA-4 Anisotropic Optical Properties of $GdScO_3$**, ***Prabin Dulal****, E. Miller,* University of Toledo*; D. Sotir, M. Barone, D. Schlom,* Cornell University*; N. Podraza,* University of Toledo

$GdScO_3$ is a wide-band gap semiconductor with a high dielectric constant, the potential to replace SiO_2 in silicon-based transistors, and use as a substrate for epitaxial thin film growth. It has an orthorhombic crystal structure resulting in crystallographic and optical anisotropy. The optical properties in the form of complex dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) spectra for each principal direction of single crystal $GdScO_3$ are investigated using generalized spectroscopic ellipsometric spectra collected over the photon energy range from 0.70 to 8.50 eV. Multiple sets of generalized ellipsometric spectra are collected from (001) and (110) surface plane oriented single crystals of $GdScO_3$ as a function of rotation about the surface normal. A divided spectral range analysis is used to determine the structural parameters of the $GdScO_3$ including bulk and surface layer thicknesses and the azimuthal Euler angle for each measurement while the remaining Euler angles are fixed based on known lattice parameters and the respective surface plane cut. In divided spectral range analysis, the full measured spectra range is subdivided into nominally transparent, weakly absorbing, and highly absorbing regions. A common structural model is used to describe the transparent and the highly absorbing spectral region to obtain common structural parameters while separate physically realistic models are applied to describe spectra in ε in each direction and both of these spectral regions. The weakly absorbing region is initially ignored as the line shape describing ε is not initially known. After obtaining structural parameters, numerical inversion is then used to extract ε corresponding to electric fields oscillating parallel to each crystallographic axis over the full spectral range, including the initially ignored weakly absorbing region. Critical points transition in ε corresponding to each direction are identified by simultaneously fitting each numerically inverted spectra in ε_2 and $d\varepsilon_2/dE$ using a sum of critical point parabolic band (CPPB) oscillators. A piecewise parameterization is developed that includes an Urbach tail below the band gap energy and CPPB behavior at and above the band gap energy to parameterize the numerically inverted optical response. The lowest direct transition is identified at 6.46 eV for electric fields oscillating parallel to a-axis, and above gap critical transitions at 6.72, 6.78, 6.95, 7.40, 7.92, and 8.25 eV are identified from all spectra in ε.

3:00pm **EL1+TF-MoA-5 Combined Density Functional Theory and Spectroscopic Ellipsometry Studies of Anisotropic Materials**, ***Rafal Korlacki**, M. Hilfiker, M. Stokey, M. Schubert,* University of Nebraska-Lincoln

INVITED

The ability of spectroscopic ellipsometry (SE) to resolve all components of the dielectric tensor combined with the predictive power of density functional theory (DFT) and related first-principles methods, is a particularly useful combination of techniques to study anisotropic materials. In recent years, a wide-bandgap gallium oxide Ga_2O_3 is a promising candidate for applications in high-power electronic devices. The most stable *β* phase, which can be grown as a high-quality bulk crystal is highly anisotropic, thanks to the low-symmetry monoclinic lattice [1,2]. In order to further increase the bandgap, the alloys of gallium oxide and aluminum oxide, $(Al_xGa_{1-x})_2O_3$, can be epitaxially grown on gallium oxide substrates. Heteroepitaxial films are inherently strained. The dependence of material properties on the components of the strain tensor for monoclinic crystals have been obtained from symmetry analysis [3], and the linear deformation potentials for energies of phonon modes and band to band transitions in Ga_2O_3 - from DFT calculations [3,4]. The same principle can be applied to the monoclinic phase of Al_2O_3, and Vegard's rule can then be used to construct a simple universal model of strain and composition dependencies of various material properties, including band-to-band transitions, refractive indices, components of the dielectric tensors, and effective mass parameters. Thus, these dependencies can be fully resolved for actual heterostructures under specific strain patterns [5,6].

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