Parameterization of the optical function of hydrogenated amorphous carbon by means of B-splines

9:40am **AS+EM+MS+TF-TuM6 VUV Optical Properties of III-Nitrides in the Thin Film Limit**, ***C. Cobet***, *M. Röppischer, C. Werner*, Institute for Analytical Sciences, Germany, *R. Goldhahn*, Ilmenau University of Technology, Germany, *N. Esser*, Institute for Analytical Sciences, Germany

In the last few years no other class of semiconductors has attracted so much scientific and simultaneously commercial attention like the group III-nitrides. The extraordinary physical properties have stimulated many new developments of (opto-)electronic devices. Prominent examples are the short wavelength laser diodes, which take advantage of the wide band gap of GaN (3.42eV). Such devices consist of three compounds: InN, GaN, AlN and their ternary or quaternary alloys. The respective band gap shifts from the near infrared for pure InN (0.68eV) to the ultraviolet for AlN (6.03eV), while the lattice constant variation is relatively small and allows the growth of heterostructures. It is probably surprising that several fundamental physical properties are still under discussion, although the III-nitrides are already widely used. Uncertainties concern, for example, the question whether zinc blende AlN has an indirect band gap or the impact of electric fields and strain on the electronic band structure. The latter effects are significant in particular for thin films, quantum wells, and super lattice structures. Furthermore, quantum size effectsalter the optical properties of such structures. But, also the knowledge about the bulk optical properties above the fundamental band gap is still incomplete.

We apply broad band spectroscopic ellipsometry from the visible to the vacuum ultraviolet. It is an excellent method in order to study electronic band structure peculiarities by means of dipole transition features in the dielectric function. On the other hand, it also allows a very precise determination of the dielectric function itself (refractive index and absorption). Device performance critically depends on the optical properties around e.g. the emission wavelength. However, this spectral region is strongly influenced by all higher inter band transitions according to the Lyddane-Sachs-Teller relation. For our investigations on binary GaN and AlN, as well as on ternary $Al_xGa_{1-x}N$, we have mainly used a home made synchrotron ellipsometer. The extraordinary properties of the synchrotron light source allow measurements with very high spectral and spatial resolution in a very broad spectral range. By taking advantage of the polarization sensitivity, we could determine the independent ordinary and extraordinary dielectric function in the hexagonal materials. In a comprehensive discussion of the dielectric functions for the hexagonal and cubic crystal structure, we could identify band gap related excitons and all higher interband transitions. This knowledge is used in order to study effects of composition and strain, as well as quantum size effects in more detail.

10:40am **AS+EM+MS+TF-TuM9 Parameterization of the Optical Function of Hydrogenated Amorphous Carbon by Means of B-splines**, ***J.W. Weber***, *T.A.R. Hansen, M.C.M. van de Sanden, R. Engeln*, Eindhoven University of Technology, The Netherlands

Spectroscopic ellipsometry (SE) is a non-invasive optical diagnostic that measures the change in polarization of light reflected on a thin film. To extract both the optical function and thickness of the film from SE data, a (multi-layered) model is required that describes the interaction of the incident light with the film. For amorphous materials this interaction is commonly modeled by the Tauc-Lorentz oscillator and is used to parameterize the optical function [1].

However, a fully mathematical Kramers-Kronig consistent description of the optical function by means of B-splines is also possible [2]. The B-spline parameterization requires no pre-existing knowledge about the interaction of light with the film. The layer structure for this model consists of a substrate, the bulk layer, of which the optical function is represented by B-splines, and a roughness layer. The roughness is modeled by an effective medium approximation of 50% bulk material and 50% voids. This layer structure is verified by cross-sectional scanning electron microscopy (SEM) measurements. The roughness is in good agreement with values determined by atomic force microscopy (AFM).

When the B-spline model is applied to SE data obtained during growth, it has been found that the optical function for every measured thickness is the same, thereby ascertaining the homogeneity of the bulk layer of the *a*-C:H. During etching of *a*-C:H with a hydrogen plasma, the optical function of the film - due to the homogeneity of the bulk material - can be fixed throughout the entire etch process, which enables real time *in situ* monitoring of the thickness evolution.

Further parameterization of the dielectric function, as found by the B-spline model, by a physics-based model is possible. For *a*-C:H films, the bulk layer is described by two Tauc-Lorentz oscillators, from which the sp^2/sp^3 ratio has been, tentatively, determined from SE data up to 6.5 eV [3].

In all, the B-spline model is an accurate and fast method to determine thickness, roughness and optical constants for numerous types of thin films, including - as has been shown - hydrogenated amorphous carbon. The determined film properties can also be used as input parameters for physics-based models.

[1] G.E. Jellison and F.A. Modine Appl. Phys. Lett.69 (1996) 371

[2] B. Johs and J.S. Hale, Phys. Stat. Sol. A **205** (2008) 715

[3] S. Kassavetis et al., Diamond Relat. Mater.16 (2007) 1813

11:00am **AS+EM+MS+TF-TuM10 Characterization of P3HT Anisotropic Thin Films with Spectroscopic Ellipsometry**, ***J.N. Hilfiker***, *J. Sun, T.E. Tiwald, G.K. Pribil*, J.A. Woollam Co., Inc.

Many methods have been developed to enhance the information content from spectroscopic ellipsometry (SE) measurements. This has allowed precise characterization of dielectrics, semiconductors, and even thin metal films. Appropriate strategies for SE characterization are needed as the thin films become more complex. The thickness and index of transparent films are readily determined. Absorbing films require additional information to uniquely determine thickness and complex refractive index. SE methods for absorbing films include interference enhancement, multi-sample analysis, optical constant parameterization, and simultaneous analysis of SE and intensity-based optical measurements.

P3HT is both absorbing across the visible spectrum and anisotropic. The anisotropy is due to molecular stacking and results in a difference between the complex refractive index parallel to the surface (in-plane) and normal to the surface (out-of-plane). To precisely characterize P3HT films requires determination of film thickness and both in-plane and out-of-plane complex refractive indices. The methods developed for absorbing films are applied to a series of P3HT thin films prepared with multiple thicknesses and on multiple substrate types.

Thick SiO_2 coatings on silicon provide interference enhancement which modifies the light-interaction in the P3HT layer as angle of incidence changes. Characterization is compared with different underlying SiO_2 thicknesses. Multi-sample analysis increases measurement information by combined analysis of samples with a common set of P3HT optical constants. This is applied to P3HT films with different thickness, as well as films coated on different substrates. The combination of SE and intensity-based measurements provides additional information about absorbing films. For P3HT coatings on glass, normal incidence transmittance can provide additional sensitivity to the in-plane complex refractive index. Optical constant parameterization reduces the solution-space, commonly restricting the optical constant functions to be smooth, continuous and Kramers-Kronig consistent. These methods are compared for P3HT films with a discussion of both merits and limitations.

11:20am **AS+EM+MS+TF-TuM11 Analysis of CdTe and CdS Thin Films and Photovoltaic Device Structures by Spectroscopic Ellipsometry**, ***M.N. Sestak***, *J. Li, J. Chen, C. Thornberry, D. Attygalle, R.W. Collins*, University of Toledo

The techniques of in-situ real-time and ex-situ spectroscopic ellipsometry (SE) have been applied for the analysis of polycrystalline II-VI thin films and device structures fabricated by magnetron sputtering onto various substrates for photovoltaics (PV) applications. The CdS/CdTe heterojunction PV technology has led to efficiencies as high as 14% (for an all-sputtered device), and to the lowest module manufacturing costs in the PV industry (< $1/W). In our SE studies, depositions of individual CdTe, CdS, and $CdTe_{1-x}S_x$ films on smooth crystalline silicon substrates have provided information on the nature of thin film nucleation and coalescence, as well as on the evolution of the dielectric function with thickness and quantum size effects in very thin films (< 30 nm). Films remain sufficiently smooth to a thickness of ~ 50 nm under a wide range of deposition conditions so that accurate dielectric functions could be determined as a function of temperature upon suspending the deposition at this thickness and cooling the film to room temperature. Such dielectric functions are deemed accurate because they are measured in situ under high vacuum, thus avoiding surface oxidation and contamination. In addition, surface roughness corrections are made based on roughness determinations obtained from the full real time SE data set. Variations with deposition conditions in the critical point parameters of the resulting room temperature CdTe and CdS dielectric functions have provided information on film stress, defects, and grain size. Upon reheating the film to the deposition temperature and resuming the deposition for the fabrication of the thick (~ 1 micron) films used in PV devices, surface roughness evolution and void volume fraction depth profiles have been extracted. These provide key insights into the optimization of a subsequent CdTe processing step – an anneal in $CdCl_2$ vapor which promotes grain growth and strain relaxation in the active CdTe layer for high efficiency PV devices. Ex situ ellipsometry techniques have also been developed that involve smoothening the thick CdTe film with a succession of $Br+CH_3OH$ treatments that enables step-by-step etching and time reversed spectroscopic ellipsometry on $CdCl_2$ treated device structures. Finally, through-the-glass SE has been developed for multilayer analysis of completed PV devices with the potential for scale up