Spectroscopic Ellipsometry Focus Topic
Room: 101 A - Session EL+AS+EN+PS+SS+TF-ThM

Spectroscopic Ellipsometry for Photovoltaics and Instrument Development

Moderator: M. Creatore, Eindhoven University of Technology, Netherlands

8:00am **EL+AS+EN+PS+SS+TF-ThM1 Application of Spectroscopic Ellipsometry for the Characterization of Various Solar Cell Devices**, ***H. Fujiwara***, Gifu University, Japan **INVITED**

To establish new structural characterization methods for Si-based and $CuInGaSe_2$(CIGS)-based solar cells, we have developed spectroscopic ellipsometry (SE) techniques that can be applied for the analysis of various textured structures used in the solar cell devices. In particular, our SE analyses allow the structural characterization of (i) hydrogenated amorphous silicon (a-Si:H) and microcrystalline silicon (μc-Si:H) tandem-type solar cells, and (ii) a-Si:H/crystalline Si (c-Si) heterojunction solar cells, both fabricated on textured substrates. For the determination of a-Si:H and μc-Si:H properties, optical databases in which the optical constants of a-Si:H and μc-Si:H are described by micro-structural factors have been constructed.[1,2] Furthermore, by developing a new optical model, we have confirmed that the high-precision analysis of a-Si:H/μc-Si:H multilayer stacks can be performed even on textured substrates having sub-micron size rough surface. On the other hand, to determine the thickness and properties of a-Si:H layers incorporated into textured a-Si:H/c-Si solar cells, SE with a tilt angle measurement configuration[3,4] has been employed. In this technique, samples are tilted so that the specular light reflection on the texture facets is measured. From this technique, we have succeeded in characterizing the properties of quite thin a-Si:H layers (5 nm) on the c-Si textures. Recently, we have applied the SE technique further to establish the structural characterization method for CIGS-based solar cells.[5] For the SE analysis, we have constructed an optical database in which the CIGS dielectric function can be calculated as functions of the Ga composition x=Ga/(In+Ga) and Cu composition y=Cu/(In+Ga). By using the constructed optical database, we have demonstrated that the structure and compositions of CIGS-based thin films can be determined accurately.

1) Kageyama et al., Phys. Rev. B 83, 195205 (2011), 2) Yuguchi et al., J. Appl. Phys. 111, 083509 (2012), 3) Saenger et al., Thin Solid Films 518, 1830 (2010), 4) Watanabe et al., Appl. Phys. Express 3, 116604 (2010), 5) Minoura et al. J. Appl. Phys. 113, 063505 (2013).

9:00am **EL+AS+EN+PS+SS+TF-ThM4 Real-Time and Through-the-Glass Mapping Spectroscopic Ellipsometry for Analysis of CdS/CdTe Coated Superstrates and Correlations with Solar Cell Performance**, ***P. Koirala***, *J. Chen, X. Tan, R.W. Collins*, The University of Toledo

In-situ real-time spectroscopic ellipsometry (RT-SE) from the film side has been applied along with ex-situ spectroscopic ellipsometry through the glass (TG-SE) toward the analysis of the different stages of CdS/CdTe solar cell fabrication in the superstrate configuration. The RT-SE studies of the CdS and CdTe layers deposited on transparent conducting oxide (TCO) coated glass superstrates provide information on the CdS growth, its surface roughness evolution, as well as overlying CdTe interface formation and bulk layer growth. Such information is very useful for developing a realistic optical model for the as-deposited layer structure in TG-SE mapping analysis over the full 15 cm x 15 cm superstrate area. In the mapping analysis, a mask is used to measure all 256 points where 0.125 cm^2 area dot cells are to be made. Because the as-deposited superstrate/film-structure undergoes additional processing steps, however, in order to complete the solar cell devices, three sets of TG-SE data maps are collected that characterize the superstrate/film-structure in the (i) as-deposited, (ii) $CdCl_2$-treated, and (iii) back-contact patterned states. With the optical database that has been established for both the as-deposited and $CdCl_2$ treated CdS and CdTe, each of the three TG-SE data maps has been analyzed based on an optical model deduced from RT-SE studies of the CdS and CdTe depositions. By using these SE techniques, we have been able to quantify the spatial dependence of the changes that occur in the superstrate/film-structure as a result of the different processing steps. In order to corroborate the layer structure determined by TG-SE, comparisons with cross-sectional transmission electron microscopy (XTEM) have been performed for selected states of the superstrate/film-structure and for selected locations. The results have been found to validate the overall RT-SE and TG-SE approach and analysis results. Finally, the layer parameters as determined from the TG-SE analyses have been correlated statistically with the device performance of the 256 dot cells fabricated over the final 15 cm x 15 cm superstrate/film-structure. The resulting correlations expedite solar cell optimization.

9:20am **EL+AS+EN+PS+SS+TF-ThM5 Expanded Beam Spectroscopic Ellipsometry for In-line Monitoring of Thin Film Process**, ***M. Fried***, Hungarian Academy of Science, Hungary **INVITED**

Non-destructive analysing tools are needed at all stages of thin film process-development, especially photovoltaic (PV) development, and on production lines. In the case of thin films, layer thicknesses, micro-structure, composition, layer optical properties, and their uniformity are important parameters. An important focus is to express the dielectric functions of each component material in terms of a handful of wavelength independent parameters whose variation can cover all process variants of that material. With the resulting database, spectroscopic ellipsometry coupled with multilayer analysis can be developed for on-line point-by-point mapping and on-line line-by-line imaging.

This talk will try to review the investigations of different types of PV-layers (anti-reflective coating, transparent-conductive oxide (TCO), multi-diode-structure, absorber and window layers, backreflector) showing the existing dielectric function databases for the thin film components of CdTe, CIGS, thin Si, and TCO layers.

Off-line point-by-point mapping can be effective for characterization of non-uniformities in full scale PV panels in developing labs but it is slow in the on-line mode when only 15 points can be obtained (within 1 min) as a 120 cm long panel moves by the mapping station. Last years [1, 2], a new instrumentation was developed that provides a line image of spectroscopic ellipsometry (wl=350-1000 nm) data. Upto now a single 30 point line image can be collected in 10 s over a 15 cm width of PV material [3, 4]. This year we are building a 30 and a 60 cm width expanded beam ellipsometer which speed will be increased by 10 X. Then 1800 points could be mapped in a 1 min traverse of a 60*120 cm PV panel or flexible roll-to-roll substrate. Another enhancement is the switch-over to rotating compensator measuring principle.

[This work was supported by the ENIAC E450EDL and KMR_12_1_2012_0225 projects]

[1] C. Major, G. Juhasz, Z. Horvath, O. Polgar, M. Fried, *PSS (c)*, **5**, 5 (2008).

[2] G. Juhász, Z. Horváth, C. Major, P. Petrik, O. Polgar and M. Fried, *PSS(c)*, **5**, 5 (2008).

[3] M. Fried, G. Juhász, C. Major, P. Petrik, O. Polgár, Z. Horváth, A. Nutsch, *Thin Solid Films***519**, 2730 (2011).

[4] M. Fried, G. Juhasz, C. Major, A. Nemeth, P. Petrik, O. Polgar, C. Salupo, Lila R. Dahal, R. W. Collins, *Mater. Res. Soc. Symp. Proc.***Vol. 1323,** DOI: 10.1557/opl.2011.820. (2011).

10:40am **EL+AS+EN+PS+SS+TF-ThM9 Materials Characterization using THz Ellipsometry and THz Optical Hall Effect**, ***T. Hofmann***, University of Nebraska-Lincoln **INVITED**

Ellipsometry in the THz spectral range has been demonstrated to be a very versatile tool for the investigation of semiconductor heterostructures, meta-materials, 2D electron gases (2DEG), and even graphene.

In this talk, instrument development with particular emphasis on frequency-domain, rotating optical element THz ellipsometry will be reviewed and recent progress on THz optical Hall-effect systems, which encompasses generalized ellipsometry in magnetic fields, will be discussed.

The application of THz ellipsometry for the accurate measurement of complex optical constants of isotropic and anisotropic bulk materials and thin films will be illustrated briefly. The progress on THz generalized ellipsometry investigations of 3D metal nanostructured thin films will be reported in detail. The investigated films exhibit a strong anisotropic optical response in the THz spectral range. It will be demonstrated that the anisotropic optical response of 3D nanostructures changes drastically as the function of the dielectric properties of the ambient. Applications for 3D metal nanostructured thin films as THz optical sensors will be discussed.

In addition, recent results on application of THz optical Hall-effect measurements will be reported. Exemplarily, temperature-dependent THz optical Hall-effect investigations of AlGaN/GaN high electron mobility transistors structures are shown. Our findings indicate that the 2DEG sheet density is independent of the sample temperature. The mobility and effective mass, however, strongly depend on the sample temperature. The mobility shows a strong increase with decreasing temperature largely due to the reduction of LO phonon scattering. The opposite behavior is observed for the effective mass and explained by the reduction of the 2DEG

confinement, i.e., the wave function penetration of the AlGaN with increasing temperature.

11:20am **EL+AS+EN+PS+SS+TF-ThM11 A History of Early Ellipsometry and Polarimetry**, ***R.A. Synowicki***, J.A. Woollam Co., Inc.

This work surveys the early history of polarimetry and ellipsometry. Special consideration is given to the time period between Drude's original work in the late 1880's and the work of Rothen in the mid 1940's.

Snell determined the refractive index of water in 1621. Isaac Newton followed in the 1660's with the prism minimum deviation technique. In the late 1880's August Kundt measured the optical properties of very thin metal films by minimum deviation, but a better technique was needed for absorbing materials.

The polarimeter was invented around 1840. Early polarimetry was used to measure the rotation of polarized light through solutions of sugar, and used in customs offices at seaports for taxation of sugar shipments. In 1845 the Faraday effect showed rotation of polarization by a magnetic field, a result later explained by James Clerk Maxwell's electromagnetic theory.

Paul Drude applied Maxwell's theory to describe the internal structure of materials. To experimentally determine optical properties Drude developed ellipsometry as an analytical technique between 1885 and 1890. Null ellipsometry techniques were originally used, but in the following decades half-shade techniques with improved accuracy became common.

Ellipsometry remained a popular technique after the time of Drude. A surprising amount of this early ellipsometry work was spectroscopic. By 1910 R.S. Minor, A.Q. Tool, and L.R. Ingersoll used ellipsometry to determine the optical constants of metals over a wide spectral range from 226 nm in the ultraviolet to 2250 nm in the infrared.

11:40am **EL+AS+EN+PS+SS+TF-ThM12 Vibrational Properties of Lanthanum Aluminate and Magnesium Aluminate Spinel Using Fourier Transform Infrared Ellipsometry**, ***T. Willett-Gies***, New Mexico State University, *C.J. Zollner,* Cornell University, *E. DeLong, S. Zollner*, New Mexico State University

Using FTIR ellipsometry, we have determined the dielectric function of twinned single-crystalline lanthanum aluminate ($LaAlO_3$) and spinel ($MgAl_2O_4$) wafers which are often used as substrate materials for oxide epitaxy. Measurements were taken at 300 K in the region of lattice vibrations between 250 and 1000 cm^{-1}. $LaAlO_3$ is a rhombohedrally distorted perovskite with two formula units per unit cell, leading to eight IR-active phonon modes [1]. Two of these eight are below our spectral range, one is very weak, and two are nearly degenerate [1]. We thus expect four TO peaks in the imaginary part of the dielectric function. The polar character of $LaAlO_3$ also causes strong LO-TO splittings. Unlike previously published FTIR reflectance studies (which require a Kramers-Kronig analysis to determine the TO/LO phonon peaks), our FTIR ellipsometry measurements allow the direct determination of TO and LO phonon energies as peaks in the dielectric function ε and the loss function 1/ε, respectively.

Magnesium aluminate spinel ($MgAl_2O_4$) belongs to the cubic O_h^7 space group and has two formula units per primitive cell. Of its 39 optic modes, factor group analysis [2] shows that there are only four IR-active modes with T_{1u} symmetry. The lattice dynamics of spinel has long been controversial and differences have been found between natural crystals (which are believed to be fully ordered) and synthetic crystals (which often contain a small amount of Mg/Al disorder).

A good description of the dielectric functions of these materials can be found using a sum of Lorentz oscillators (for the TO phonons in our spectral range) and two poles for electronic and low-energy phonon absorption outside of our spectral range. A factorized model [3] with LO/TO phonon pairs and a UV pole yields even better agreement with the data. The classical Lorentz model assumes a frictional force proportional to the velocity of the atoms resulting in a single broadening parameter, while the Lowndes model [3] takes into account the anharmonic phonon decay and assigns independent broadening parameters to the LO and TO phonons. Our FTIR ellipsometry measurements yield LO and TO parameters (energies, broadenings, and oscillator strengths) with unprecedented accuracy, far exceeding those from previous FTIR reflectance results. We will compare our experimental phonon energies with those obtained from *ab initio* density-functional theory for both $LaAlO_3$ and $MgAl_2O_4$.

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[2] A. Chopelas and A.M. Hofmeister, *Phys. Chem. Minerals***18**, 279 (1991).

[3] R. P. Lowndes, *Phys. Rev. B***1**, 2754 (1970).

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