DS 9: Layer Properties: Electrical, Optical, and Mechanical Properties

Time: Tuesday 9:30–12:45 Location: CHE 91

Invited Talk DS 9.1 Tue 9:30 CHE 91

Chalcopyrite semiconductors: atomic-scale structure and band gap bowing — •Claudia S. Schnohr[1], Stefanie Eckner[1], Helena Kämmer[1], Tobias Steinbach[1], Martin Gnauck[1], Andreas Johannes[1], Christian A. Kaufmann[2], Christiane Stephan[2], and Susan Schorr[2] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

$Cu(In,Ga)Se_2$ is one of the most promising material systems for thin film photovoltaics with record efficiencies above 20% on laboratory scale. The material crystallizes in the chalcopyrite type crystal structure where the anion is typically displaced from its ideal lattice site due to the different properties of the neighbouring cations. This subtle structural variation has a strong influence on the energy band gap. Therefore, we have studied the atomic-scale structure of $Cu(In,Ga)Se_2$ as a function of composition using extended X-ray absorption fine structure spectroscopy and valence force field simulations. The local atomic arrangements are found to deviate significantly from the long-range crystallographic structure and the material is characterised by structural inhomogeneity on the atomic scale. Regarding the anion position, two different displacement mechanisms have to be distinguished both of which influence the nonlinear change of the band gap with material composition. Similar results were also obtained for $Cu(In,Ga)S_2$ indicating that our findings represent general features of these highly relevant yet complex chalcopyrite semiconductors.

Invited Talk DS 9.2 Tue 10:00 CHE 91

Polarized mid-infrared spectroscopy of split-ring resonators and metal nanoparticle-organic hybrids — •Thomas W.H. Oates, Dimitra Gkogkou, Timur Shaykhutdinov, Tolga Wagner, and Karsten Hinrichs — Leibniz-Institut für Analytische Wissenschaften - ISAS- e.V., Albert-Einstein Str. 9, 12489, Berlin, Germany

Metal nano-antennas are increasingly utilized to focus the electric far-field, with the goal of enhancing and manipulating interactions with organic resonators in the near-field. In the infrared spectral fingerprint region, the use of polarized infrared spectroscopy provides unique information concerning the 3D orientation of the resonant structures. We present the results of ellipsometry and polarized infrared microscopy investigations of an array of split-ring resonators (SRR) and metal nanoparticle (NP) films with adsorbed self-assembled monolayers. The SRRs show an extrinsic chiral response directly related to the combined symmetry of the metallic structures and the electric field of the incident radiation. Rigorous coupled wave analysis simulations give excellent agreement with the experimental results. The polarized reflection spectra of the metal NP-organic hybrids display surface-enhanced infrared absorption (SEIRA). Using a combinatorial fabrication method we produce an array of nanoparticle sizes, shapes and fill-factors on a single substrate. This allows us to precisely identify the optimal conditions for maximal SEIRA enhancement. The additional information provided by polarized spectroscopy allows us to discuss the origins of the SEIRA effect.

DS 9.3 Tue 10:30 CHE 91

Investigations of the dependency of the infrared-optical and electrical properties of ITO coatings on the dip coating parameters and the coating thickness — •Nadine Wolf, Thomas Weis, and Jochen Manara — Bavarian Center for Applied Energy Research (ZAE Bayern)

Tin doped indium oxide (ITO) coatings were prepared with ITO nanoparticle suspensions via dip coating technique. The coatings have been prepared with different withdrawal speeds so that the coatings exhibit different thicknesses. If the thickness of the ITO coatings increases, the amount of free charge carriers within these coatings also increases and therefore the infrared-optical and electrical properties of the ITO coatings alter up to a certain extent, too. The change of the thickness and the optical constants of the ITO coatings with the withdrawal speed are measured with ellipsometry measurements. The infrared-optical and electrical properties are measured with Fourier transform infrared (FTIR) spectroscopy and four point probe measurements respectively. In this work the dependency of these properties is discussed as a function of the thickness and therefore withdrawal speed.

DS 9.4 Tue 10:45 CHE 91

Sputter yield amplification upon reactive serial co-sputtering of doped TiO2 — •Rüdiger M. Schmidt[1], Tomas Kubart[2], Andreas Pflug[3], and Matthias Wuttig[1,4] — [1]I. Institute of Physics, RWTH Aachen University, Germany — [2]Solid State Electronics, The Ångström Laboratory, Uppsala University, Sweden — [3]Fraunhofer IST, Braunschweig, Germany — [4]JARA - Fundamentals of Future Information Technologies

TiO_2 plays a prominent role in several applications such as anti-reflective coatings and self-cleaning surfaces, mainly because of its high refractive index. Most frequently this material is deposited by reactive magnetron sputtering. Unfortunately TiO_2 suffers from a comparatively low deposition rate. To increase the deposition rate, Sputter Yield Amplification (SYA) can be used through recoil of the sputtering species at implanted heavy dopants below the target surface. Here we present experimental results for different heavy dopants using a dedicated sputter deposition tool. By use of serial co-sputtering in situ variations of the target stoichiometry can be facilitated, which enable systematic studies of SYA. To quantify the amplification, film thicknesses have been deduced by x-ray reflectometry measurements and subsequent simulations. Ellipsometry as well as reflectance and transmission data have been taken to model the dielectric function of the resulting films giving access to the refractive index.

DS 9.5 Tue 11:00 CHE 91

Sponge-like Si-SiO2 nanocomposite as photovoltaic absorber * influence of composition of the SiOx precursor — •Erik Schumann[1], Karl-Heinz Heinig[1], René Hübner[1], Jose Luis Endrino[2], and Gintautas Abrasonis[1] — [1]Helmholtz-Zentrum Dresden, Rossendorf, Dresden, Germany — [2]Abengoa Research, Sevilla, Spain

Absorber layers consisting of nanostructured Si are candidates to improve the efficiency of thin film Si solar cells. Si-SiO2 nanocomposites with sponge-like Si embedded in SiO2 are promising materials as they exhibit a widened band gap and maintain the electrical interconnectivity. These structures can be formed upon annealing of SiOx films (x<1), which leads to spinodal phase separation into a percolacated network of Si nanowires embedded in SiO2. This can be accompanied by crystallization of the silicon. The influence of the composition of the precursor SiO2 on the evolving sponge-like nanostructure is investigated. SiOx layers have been grown by reactive sputter deposition. SiOx layers with compositions between x=0 and x=1.2 have been studied. The transformation of SiOx into Si-SiO2 nanocomposites has been performed by scanning a diode laser line source. Dwell times in the ms range and power densities of the red laser light of about 103 W/cm2 have been investigated. While thin a-Si films show crystallization under our annealing conditions, oxygen-rich films with Si structures smaller than 2 nm do not crystallize. Our results demonstrate that the composition of the precursor material is of crucial importance to obtain a Si-SiO2 nano sponge-like material suitable as photovoltaic absorber.

Coffee break (15 min)

DS 9.6 Tue 11:30 CHE 91

The Origin of the Radial Distribution of the Electronic and Structural Properties of Magnetron Sputtered ZnO:Al Thin Films — •André Bikowski[1], Thomas Welzel[2], and Klaus Ellmer[1] — [1]Helmholtz-Zentrum Berlin, D-14109 Berlin — [2]Technische Hochschule Mittelhessen, D-35390 Gießen

We investigated the electronic and structural properties of magnetron sputtered ZnO:Al films by means of radially resolved X-ray diffraction, resistivity, and plasma process monitor measurements.

It is known for a long time now that films sputtered onto stationary substrates exhibit a pronounced radial distribution of their electronic and structural properties. Mainly there exist two explanations for this effect: (i) The inhomogeneities are caused by excess oxygen reaching the substrate surface or (ii) they are due to a bombardment of the growing films by high energetic oxygen.

We were able to clearly correlate the radially resolved ion energy distribution spectra of high energetic negative oxygen ions to the electronic and structural properties of the films, and hence found model (ii) to be more appropriate. Since these high energetic negative ions exhibit energies in the range of several hundred eV in the case of DC sputtering, and the formation energies of defects in ZnO are some 10 eV only, a strong impact of the high energetic ions on the structural and the related electronic properties is to be expected. Generally, the results show a decisive role of high energetic oxygen for magnetron sputtering, which has to be taken into account also for other TCO materials such as In_2O_3:Sn or SnO_2:F.

DS 9.7 Tue 11:45 CHE 91

Structural and Electrical Characterization of the Ferecrystals $[(PbSe)_{1.14}]_m(NbSe_2)_n$ — •Corinna Grosse[1], Matti Alemayehu[2], Olivio Chiatti[1], Anna Mogilatenko[1], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA

Ferecrystals are layered intergrowth compounds consisting of alternating few-atomic-layers thin sheets of transition metal dichalcogenide (TMD) and metal chalcogenide layers. TMDs exhibit interesting electrical properties such as charge density waves, superconductivity or an ultralow thermal conductivity [1]. In contrast to conventional misfit layer compounds, ferecrystals exhibit a turbostratically disordered structure and their layer thickness and stacking sequence are tunable.

In this study, we synthesized the ferecrystals $[(PbSe)_{1.14}]_m(NbSe_2)_n$ and measured their in-plane electrical properties as a function of layer sequence (m and n) and temperature (down to $T = 300$ mK). The crystal structure was analyzed using X-ray- and electron diffraction, scanning transmission electron microscopy and energy-dispersive X-ray spectroscopy. The structure of the PbSe and $NbSe_2$ constituents was resolved down to the atomic scale. The influence of the ferecrystal structure on the electrical properties is discussed. [1] C. Chiritescu, D. G. Cahill, N. Nguyen, D. C. Johnson *et al.*, Science **315**, 351 (2007).

DS 9.8 Tue 12:00 CHE 91

Effect of temperature on the electrical and mechanical performance of Al-Li thin films deposited on viscoelastic substrates — •Alla S. Sologubenko, Diana Courty, and Ralph Spolenak — Laboratory for Nanometallurgy (LNM), ETH Zurich, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich, Switzerland

Grain boundary cohesion and adhesion of the metallic thin film to a polyimide substrate are two factors crucially affecting the structural integrity of Al-Li alloys upon tensile loading. Al-Li thin film alloys of different compositions and microstructures were subjected to mechanical loading experiments accompanied by electrical resistance measurements in a tensile stage equipped with an in-situ heating module. The experiments performed at 100°C show drastic change in both, mechanical and electrical responses of the thin films of all compositions in comparison to room temperature measurements. This behavior evidences a large enhancement of adhesion in the thin film-substrate system due to the temperature increase. The exceptionally good performance of the equisize-grained Al-5 at.%Li alloy at both temperatures is attributed to an effect of the small intermetallic phase particles on the film plasticity and grain boundary cohesion.

DS 9.9 Tue 12:15 CHE 91

Thick LCMO manganite films grown by MAD — •F. Fischgrabe[1], E.S. Zhukova[2,3], B. Gorshunov[2,3], M. Dressel[3], and V. Moshnyaga[1] — [1]I. Physikalisches Institut, Universität Göttingen, Germany — [2]Prokhorov General Physics Institute, Russian Academy of Sciences,Moscow, Russia — [3]I. Physikalisches Institut, Universität Stuttgart, Germany

We report preparation and characterization of $La_{1-x}Ca_xMnO_3$ (LCMO) x=0,5-0,96 films with thickness $0,5\mu m$. Thick epitaxial manganite films could be interesting for THz as well as for far IR Fourier spectroscopy measurements, aimed to study low-energy excitations, like CDW and folding phonons, important for the manganite physics. The samples were grown using metalorganic aerosol deposition (MAD) technique. To verify the film quality XRD, DC and AC resistivity (f=0,1Hz-40MHz; T=5-300K), STM, REM, Squid, Raman, and THz measurements were carried out. $0,5\mu m$-thick LCMO films with $x \geq 0,5$ show charge-order transitions and residual resistivity, $\rho(300K) \approx 10^{-4}\Omega cm$. The films show crossover from insulating to semiconductor-like behaviour at high temperatures. We further demonstrate drastic changes of all measured properties with increasing doping level, aswell as dependance on comensurate dopinglevels. Furthermore we present results on freestanding films also prepared by MAD technique. Preparationprocedure and first results aswell as comparison with films on MgO will be shown.

DS 9.10 Tue 12:30 CHE 91

Investigating Few Layer Gallium Selenide (GaSe) with Advanced Atomic Force Microscopy and Optical Techniques — •Matthias A. Fenner[1], Raul D. Rodriguez[2], Alexander Villabona[2,3], Santos A. Lopez-Rivera[3], and Dietrich R.T. Zahn[2] — [1]Agilent Technologies, 60528 Frankfurt, Germany — [2]Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [3]Universidad de Los Andes, Applied Physics Lab, Merida 05101, Venezuela

Gallium selenide (GaSe) nanosheets have been reported to exhibit superior properties in field effect transistors and photo detectors as compared to other two-dimensional, layered materials [1-3]. We prepared few layer GaSe flakes by mechanical transfer to a graphite substrate. Individual flakes of several tens micrometer size are obtained and can readily be detected by optical microscopy. We used atomic force microscopy to investigate the nanoscale mechanical and electrical properties of the flakes. We will discuss the remarkable differences observed in the same area investigated by Raman spectroscopy and imaging, in particular, the correlation between the first order Raman modes of GaSe and the selective enhancement of the underlying graphite substrate.

[1] P. Hu, Z. Wen, L. Wang, P. Tan, K. Xiao, Acs Nano, 6 (2012) 5988. [2] S. Lei, L. Ge, Z. Liu, S. Najmaei, G. Shi, G. You, J. Lou, R. Vajtai, P.M. Ajayan, Nano Lett., 13 (2013) 2777. [3] D.J. Late, B. Liu, J. Luo, A. Yan, H.S.S.R. Matte, M. Grayson, C.N.R. Rao, V.P. Dravid, Adv. Mat., 24 (2012) 3549.