HL 5: Photovoltaics: CIGS and related compounds

Time: Monday 9:30–11:45 Location: EW 202

HL 5.1 Mon 9:30 EW 202

Investigation of Defect Levels in Al/Cu(In,Ga)Se_2 Schottky Contacts and ZnO:Al/CdS/Cu(In,Ga)Se_2 Heterojunctions via Temperature-Dependent Admittance Spectroscopy — •Sara L. Gadeberg, Maria S. Hammer, and Ingo Riedel — Energy and Semiconductor Research Laboratory, Chair: Jürgen Parisi, Department of Physics, University of Oldenburg

Regardless their broad application and investigation, many properties of the Cu(In,Ga)Se_2 compound semiconductors (CIGSe) have still not been sufficiently explained. For instance, the nature of certain defect signatures (interface or bulk) is still under discussion. In this study different Schottky contacts (Al/CIGSe/$MoSe_2$/Mo) were prepared from CIGSe solar cells (ZnO:Al/CdS /CIGSe/$MoSe_2$/Mo) via etching removal of the ZnO:Al/CdS window layer, surface treatment of the remaining CIGSe layer, and subsequent metal deposition. In order to differentiate between bulk and heterojunction interface defects, we recorded temperature-dependent admittance spectra (TAS) (T=30 - 310 K). The TAS data were evaluated in two ways: i) by applying the common method using the derivative of the capacitance and ii) by direct analysis of the phase shift of the impedance, which does not require particular assumptions on the electrical device equivalent circuit. The defect signatures found in the Schottky devices were compared to those found in the original CIGSe solar cells. Based on our results we will discuss the spatial origin of the different defect levels and comment on the reliability of the direct evaluation method for TAS data as proposed in this work.

HL 5.2 Mon 9:45 EW 202

Influence of metastable defect characteristics on the carrier collection in Cu(In,Ga)Se_2 thin film solar cells — •Maria S. Hammer[1], Viktor Gerliz[1], Stephan J. Heise[1], Jörg Ohland[1], Janet Neerken[1], Jan Keller[2], and Ingo Riedel[1] — [1]Energy and Semiconductor Research Laboratory, Chair: Jürgen Parisi, Department of Physics, University of Oldenburg — [2]Currently: Department of Engineering Sciences, Solid State Electronics, Uppsala Universitet

Despite the current progress of Cu(In,Ga)Se_2 thin film photovoltaics, the relation between the metastable defect characteristics and key parameters of the solar cells has not yet been fully explained. In this work we discuss the correlation between metastable defect densities and short-circuit current J_{SC} of solar cells conditioned via white-light soaking (LS) and dark air-annealing (DA), respectively. The J_{SC} of DA-treated devices was found to decrease by 0.8 $mAcm^{-2}$ upon LS treatment, which suggests a conditioning-induced change of the carrier collection. Partly, this phenomenon can be attributed to a change of the metastable net doping density. However, device simulations and cross-section EBIC measurements suggest that this explanation is not sufficient to describe the observed J_{SC} difference. Moreover, time-resolved photoluminescence revealed a significant decrease of the decay lifetime upon LS along with an increase of the N1 defect concentration by $9.5{\cdot}10^{14}$ cm^{-3}, as evaluated from temperature dependent admittance spectra. In conclusion, we propose, that the observed J_{SC} metastability originates from both, treatment-induced changes of the net doping concentration and defect-related transport properties.

HL 5.3 Mon 10:00 EW 202

Kinetics of phase separation and coarsening in Cu-In-Ga precursor thin films for sequentially processed Cu(In,Ga)Se_2 solar cells — •Jan-Peter Bäcker[1], Humberto Rodriguez-Alvarez[1], Manuel Hartig[3], Christian A. Kaufmann[1], Jaison Kavalakkatt[2], Roland Mainz[2], Saoussen Merdes[1], Sebastian S. Schmidt[1], Christian Wolf[1], Florian Ziem[1], and Rutger Schlatmann[1] — [1]PVcomB, Helmholtz-Zentrum Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Technische Universität Berlin, Germany

Obtaining smooth and homogenous Cu(In,Ga)Se_2 films by fast selinzation of metallic precursors is a major challenge. Separation and coarsening of metallic phases in Cu-In-Ga precursor films can lead to solar cells with low shunt resistance due to pinhole formation, and to reduced open circuit voltages due to locally varying Ga concentration. In this study we attempt to establish a general model for the kinetics of the phase separation and coarsening of sputtered Cu-Ga-In metallic films as used for Cu(In,Ga)Se_2 fabrication. For this we measure the roughness with atomic force microscopy and the Ga spatial distribution by energy dispersive X-ray spectroscopy. We study four different metallic precursor stacks heated to 170°C, 350°C and 580°C, at rates between 0.01K/s and 1K/s. Finally, we present a statistical analysis of the effect of our optimized multilayered precursors on the fill factor of the solar cells prepared in our atmospheric-pressure in-line and fast selenization baseline, that has led to power conversion efficiencies of up to 15.5% (active area).

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A Real-Time XRD Investigation of $Cu(In,Ga)Se_2$ by Three-Stage Thermal Co-Evaporation — •Setareh Zahedi-Azad, Paul Pistor, Enrico Jarzembowski, Stefan Hartnauer, Leonard Wägele, Wolfgang Fränzel, and Roland Scheer — Institute of Physics, Martin-Luther-University Halle-Wittenberg

Solar cells based on $Cu(In,Ga)Se_2$ (CIGS) thin films have achieved efficiencies of up to 21.7%, which makes this technology comparable to Si-based Solar cells. Further improvement requires a detailed understanding of the crystal phase evolution during preparation. Therefore, the phase evolution of $Cu(In_{1-x},Ga_x)Se_2$ thin films prepared by multi-stage co-evaporation and with x (= Ga/Ga+In) ranging from 0 to 1, was investigated during the deposition process via time resolved in situ X-ray diffractometry (in situ XRD). Dependent on x, films exhibit different crystalline phases during the different stages of the growth. The phases monitored during the growth of $CuInSe_2$ (x=0) are in agreement with the $In_2Se_3 - Cu_2Se$ pseudo-binary phase diagram. In this case and in the case of x = 0.33, ordered vacancy phases of $Cu(In,Ga)_5Se_8$ and $Cu(In,Ga)_3Se_5$ are observed, while for higher Gallium contents (x>=0.55), no such phases were detected. The formation of Cu_2Se phases was observed at the beginning of the Cu-rich growth regime for all processes. The Cu_2Se diffraction peaks disappear again in the third stage when the samples become Cu-poor again. The XRD peak width is analyzed quantitatively and interpreted in terms of crystallite size, crystalline quality and compositional gradients within the layer.

HL 5.5 Mon 10:30 EW 202

Composition-dependent atomic-scale structure of the Cu-(In,Ga)-Se system — •Erik Haubold[1], Philipp Schöppe[1], Stefanie Eckner[1], Susan Schorr[2], Francesco di Benedetto[3], Ivan Colantoni[4], Francesco d'Acapito[4], and Claudia S. Schnohr[1] — [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 & Institut für Geologische Wissenschaften, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany — [3]Dipartimento di Scienze della Terra, Università degli Studi di Firenze, Via La Pira 4, 50121 Firenze, Italy — [4]European Synchrotron Radiation Facility, 6 rue Jules Horowitz, BP 220, 38043 Grenoble Cedex, France

Cu(In,Ga)Se_2 shows the highest conversion efficiencies of all thin film solar cells with more than 20%. It is believed that the formation of copper poor surface regions within the absorber is important for reaching these high efficiencies. The properties of the material, including the bandgap energy, are determined not only by the material composition and crystal structure but also by the local arrangement of atoms. Therefore, we studied the atomic-scale structure of Cu(In,Ga)Se_2 and the two copper poor phases Cu(In,Ga)$_3Se_5$ and Cu(In,Ga)$_5Se_8$ as a function of the In/Ga ratio using extended X-ray absorption fine structure spectroscopy. This yields the element-specific average bond lengths and bond length variations as a function of In/Ga ratio and Cu content thus providing a comprehensive picture of the relationship between local structural parameters and material composition.

HL 5.6 Mon 10:45 EW 202

First Principle Calculation on the Energetics of Na and K Incorporation in CuInSe2 and CuIn5Se8 — Elaheh Ghorbani[1,2], •Janos Kiss[3], Hossein Mirhosseini[3], Thomas Kuehne[4], and Claudia Felser[3] — [1]Johannes Gutenberg univesity, Mainz, Germany — [2]IBM, Mainz, Germany — [3]MPI for Chemical Physics of Solids, Dresden, Germany — [4]University of Paderborn, Paderborn, Germany

In the present work we study sodium and potassium extrinsic defects

incorporating into several substitutional and interstitial positions in CuInSe2 and CuIn5Se8 by means of theoretical density functional theory calculations (including some fraction of exact Hartree-Fock exchange). Our research reveals the most and least favorable sites for Na and K in the light absorber layer of CIGS-based thin film solar cells. We have also studied the energetics of dumbbells. Our calculations show: (i) Among substitutional positions, occupying a Cu position (by Na or K) takes much less energy than occupying an In or a Se position. (ii) Interstitial positions which are tetrahedrally coordinated by 2 Na and 2 In are more favourable for both Na and K than interstitial positions which are tetrahedrally coordinated by 4 Se atoms. (iii) All (Na-Na), (Na-K) and (K-K) dumbbells can form in CuInSe2 and CuIn5Se8. Among dumbbells (Na-Na) and (K-K) have the lowest and highest formation energies respectively. (iv) Dumbbells can occupy the pristine vacant copper position of CuIn5Se8, without creating new Cu-defects. (v)Our band structure results show which defects will cause the appearance of new defects states in the gap of absorber.

HL 5.7 Mon 11:00 EW 202

Local versus global electronic properties of chalcopyrite alloys — Rafael Sarmiento-Pérez[1], Silvana Botti[1], •Claudia S. Schnohr[2], Iver Lauermann[3], Angel Rubio[4,5], and Benjamin Johnson[5] — [1]Institut Lumière Matière, Université Lyon 1-CNRS, 69622 Villeurbanne Cedex, France — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [4]Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, Avenida de Tolosa 72, 20018 San Sebastián, Spain — [5]Fritz Haber Institute, Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Among the materials used for thin film solar cells, $Cu(In,Ga)(S,Se)_2$ has reached the highest conversion efficiencies with record values well above 20%. The bandgap energy of the material can be tailored by adjusting the In/Ga ratio which mostly affects the position of the conduction band minimum. Therefore, we have studied the element-specific unoccupied electronic states of $Cu(In,Ga)S_2$ as a function of the In/Ga ratio by combining X-ray absorption spectroscopy with ab initio calculations. The S absorption edge shifts with changing composition as expected from the variation of the band gap. In contrast, the cation edge positions are largely independent of composition. This unexpected behavior is well reproduced by our calculations and originates from the dependence of the electronic states on the local atomic environment. The variation of the bandgap arises from a changing spatial average of these localized states with changing alloy composition.

HL 5.8 Mon 11:15 EW 202

Photoreflectance and photoluminescence of Cu(In,Ga)S2 thin film solar cells — •Sergiu Levcenko, Joachim Klaer, Steffen Kretzschmar, and Thomas Unold — Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany

An increased open-circuit voltage and an improved photocurrent collection have been recently achieved in Cu(In1-x,Gax)S2 (CIGS)- thin film based cell due to properly designed gallium alloying in the absorber layer. Nevertheless, the open-circuit voltage deficiency in CIGS devices is still larger than in selenide chalcogenide-based solar cells. It is believed that recombination at CdS/CIGS interface strongly reduces the device performances.

In our study we employ the nondestructive and contactless photoreflectance (PR) and photoluminescence (PR) techniques for characterizing CIGS devices. The CIGS absorbers with Ga/Ga+In ratio of 0.27 were fabricated under copper-rich conditions by a rapid thermal process with subsequent removal of segregated CuS by KCN etching. The effect of sulfurization temperature and post deposition treatments (KCN etching, NaF, In2S3 and In thin layer extra depositions) of the absorber in CIGS devices was revealed by PR and PL measurements at a room temperature. In the near band edge region the PR spectra show distinct structures at 1.5 and 1.55eV, while the PL signal consist of a broad band at 1.5eV with full width at half maximum of 100meV. The structures in PL and PR spectra are found to be influenced by the absorber preparation parameters.

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Simulation of interference-related lineshape distortions in electroreflectance spectra of $Cu(In,Ga)Se_2$ thin-film solar cells — •Christian Huber[1], Christoph Krämmer[1], David Sperber[1], Heinz Kalt[1], Michael Powalla[2], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute, KIT and Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany

Modulation spectroscopy techniques like electroreflectance (ER) have proven to be powerful methods to determine the energetic positions of critical points (CPs) in a semiconductor's band structure. In the low-field regime the sharp, derivative-like features at the CPs can easily be evaluated by fitting a third-derivative functional form (TDFF) lineshape to the measured spectra.

However, when applied to thin-film solar cells to determine the absorber band gap, deviations from the TDFF approach have to be considered. One important aspect is that the layer stack of the solar cell introduces layer thickness interferences in the reflection signal, which can strongly distort the ER spectra.

In this contribution a transfer matrix approach will be presented in order to model the ER spectra of $Cu(In,Ga)Se_2$ thin-film solar cells. It shows that interference effects introduce lineshape distortions whenever interference minima lie energetically close to a CP. These distortions can easily be misinterpreted as contributions from several CPs and will therefore lead to wrong results in a TDFF-evaluation.