

HL 6: Photovoltaics I

Time: Monday 9:30–13:00

Location: EW 203

HL 6.1 Mon 9:30 EW 203

Formation process of the CIGSe absorber layers in a two stage sequential process — ●SVEN SCHÖNHERR, PHILIPP SCHÖPPE, MICHAEL OERTEL, UDO REISLÖHNER, and CARSTEN RONNING — Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

A sequential process is often used to produce Cu(In,Ga)Se₂ (CIGSe) solar cells, which show high efficiencies of light conversion. In our process, the metallic precursor on top of a molybdenum back contact was reactively annealed in a selenium vapour atmosphere where it is typically converted to an about 2 μm thick CIGSe absorber layer. The selenization was spilt in two stages to get a better control of the absorber formation process. Completing the solar cell, a CdS buffer layer was grown via chemical bath deposition and as front contact a ZnO layer was sputtered on top. For a more homogeneous CIGSe absorber layer we varied the substrate temperature and the selenization time in the second stage. Current-voltage and capacitance-voltage measurements were used for a first electrical characterization. X-ray diffraction were taken to investigate the phase formation in the final absorber and in the molybdenum diselenide layer at the back contact. Furthermore, thin cross section lamellas of the complete solar cell were prepared via a focused ion beam system to measure the gallium gradient via energy dispersive X-ray spectroscopy. Additionally, photoluminescence measurements at low temperatures were performed to characterize the defect structure and to get information about the ratio of group III elements.

HL 6.2 Mon 9:45 EW 203

The beneficial effect of Rubidium in Cu(In,Ga)Se₂ solar cells — ●PHILIPP SCHÖPPE¹, SVEN SCHÖNHERR¹, ROLAND WUERZ², WOLFGANG WISNIEWSKI³, GEMA MARTÍNEZ-CRIADO^{4,5}, MAURIZIO RITZER¹, KONRAD RITTER¹, CARSTEN RONNING¹, and CLAUDIA SARAH SCHNOHR¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Stuttgart, Germany — ³Otto-Schott-Institut, Friedrich-Schiller-Universität Jena, Germany — ⁴Instituto de Ciencia de Materiales de Madrid, Spain — ⁵European Synchrotron Radiation Facility, Grenoble, France

Cu(In,Ga)Se₂ solar cells are the most efficient ones among all thin film photovoltaics. The current world record efficiency was realized by applying a RbF post deposition treatment (PDT) to the absorber. However, it is not clear why the introduced Rb improves the solar cell performance. In order to investigate the beneficial effect of Rb, a Cu(In,Ga)Se₂ absorber was grown on a Mo coated alkali free substrate and subjected to a RbF PDT. This pure RbF PDT leads to a significantly higher efficiency. A thin cross sectional lamella was cut out of the layer stack and investigated via a combination of electron microscopy and synchrotron based x-ray fluorescence analysis. This approach provides clear indications of the origin of the beneficial effect of Rb. It is evident that Rb segregates at random grain boundaries and dislocation cores, where it likely passivates defects. In contrast, Rb does not segregate at Σ3 twin boundaries. Additionally, Rb agglomerates at the interface between the absorber and the MoSe₂ layer.

HL 6.3 Mon 10:00 EW 203

Computational investigation of quantum well superlattice solar cells — URS AEBERHARD¹ and ●JOSE MARIA ULLOA² — ¹IEK-5 Photovoltaik, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Institute for Systems based on Optoelectronics and Microtechnology (ISOM), Universidad Politécnica de Madrid, Ciudad Universitaria s/n, E-28040 Madrid, Spain

Quantum well superlattices (QWSL) are widely considered as tunable absorbers in high-efficiency multi-junction solar cells. In conventional models for the photovoltaic properties of QWSL, the latter is treated as an effective bulk medium with modified material parameters derived from a perfectly periodic structure, where transport is assumed to proceed in band-like fashion via extended superlattice Bloch states. In realistic implementations, deviations from this flat-band bulk picture are induced by the presence of built-in fields, scattering and disorder, as well as the finite number of periods.

We quantify these deviations using a comprehensive non-equilibrium quantum statistical mechanics approach to the computation of charge

carrier dynamics in non-idealized QWSL. By consideration of the spectral information on density of states, scattering rates and current flow, we specifically address the transition from QWSL to multi-quantum-well behavior with increasing period thickness, type-I vs type-II band alignment, the effect of the number of SL periods, as well as the impact of electron-phonon scattering, built-in fields and disorder in the heterostructure potential. The findings are related to experimental data from type-I GaAs/GaAsNSb and type-II GaAsN/GaAsSb QWSL.

HL 6.4 Mon 10:15 EW 203

Band-gap tuning of Cu₂ZnSn(S,Se)₄ solar cell absorbers via defined adjustment of the chalcogenide ratio using a post-sulphurization process — ●MARKUS NEUWIRTH¹, ELISABETH SEYDEL¹, JASMIN SEEGER¹, ALEXANDER WELLE^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH⁴ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Institute of Functional Interfaces, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen — ³Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen — ⁴Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe

Kesterite Cu₂ZnSn(S,Se)₄ (CZTSSe) thin-film solar cells are promising candidates for the future photovoltaic market. One of their very interesting and useful features is the tunability of their absorber band gap. In our work we achieve this by tuning the chalcogenide ratio $x = [S]/([S]+[Se])$ from close to 0 up to 1, which corresponds to a band-gap range of about 1.0 eV up to 1.5 eV. Experimentally this is done by post-annealing selenium-rich ($x = 0.1$) absorbers in a sulphur atmosphere. By varying the temperature and process hold time during this post-sulphurization step, we are able to accurately adjust x . Studies of the elemental composition give insight into the sulphur incorporation process which seems to be strongly correlated with the absorber's morphology before post-sulphurization. Further morphology studies and current-voltage characteristics of the solar cells show a clear trend for the dependency of the device performance on process parameters.

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Element-specific atomic-scale structure of Cu₂(Zn,Fe)SnS₄ kesterite-stannite alloys — ●CORA PREISS¹, KONRAD RITTER¹, STEFANIE ECKNER¹, PHILIPP SCHÖPPE¹, SUSAN SCHORR², and CLAUDIA S. SCHNOHR¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — ²Helmholtz-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

The chalcogenides Cu₂ZnSnS₄ (kesterite) and Cu₂FeSnS₄ (stannite) are interesting as potential photovoltaic absorbers being non-toxic and earth-abundant. In Cu₂(Zn,Fe)SnS₄, the S anions are surrounded by different local cation configurations. Therefore, Cu₂ZnSnS₄, Cu₂FeSnS₄, and their solid solutions with different Zn/(Zn+Fe) ratios were investigated with extended X-ray absorption fine structure spectroscopy. The absorption was measured at the K-edges of Cu, Zn, Sn, and Fe thus revealing the element-specific bond lengths of the material. All bond lengths are nearly independent of composition, yet they differ substantially for the different elements. While the Cu-S and Fe-S bond lengths are identical, the Zn-S and Sn-S bond lengths are larger by about ~0.03 and 0.12 Å, respectively. Based on these experimental results, the S anion position is modelled for two possible cation nearest neighbour configurations. The S position is clearly different in the Zn and the Fe containing environment, leading to an intrinsic structural inhomogeneity on the submicrometer scale.

HL 6.6 Mon 10:45 EW 203

CZTSe solar cells prepared by co-evaporation of Cu-Sn/CZTSe/ZnSe/CZTSe layer stacks — ●LWITIKO MWAKYUSA^{1,3}, MARKUS NEUWIRTH¹, ULRICH PAETZOLD³, BRYCE RICHARDS^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH² — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe — ²Light Technology Institute, (KIT), 76131 Karlsruhe — ³Institute of Microstructure Technology, (KIT), 76344 Karlsruhe

CZTSe solar cells are a promising alternative for CIGS- and CdTe-

based technologies because they only comprise non-toxic and earth-abundant elements. However, the main concern of this approach is the low conversion efficiency compared to CIGS and CdTe. Essentially, CZTSe device performance is limited by a high open-circuit voltage (V_{oc}) deficit and a low fill factor (FF). It is often assumed that this is related to a high recombination rate at the heterojunction and Mo/CZTSe interface. It has been proven that, the reaction of Mo and CZTSe promotes the formation of a thicker $MoSe_2$ layer as well as unwanted phases and defects at the interface. The latter could harm solar cell performance, especially V_{oc} , series resistance (R_s) and FF . To suppress this challenge, alloyed precursors with a configuration of Mo/Cu-Sn/CZTSe/ZnSe/CZTSe are employed in this work and compared to single-layered co-evaporated CZTSe precursors with respect to material growth and device performance. The presence of an alloyed Cu-Sn seed layer prevents earlier interaction of the CZTSe absorber with the Mo back-contact. In addition the influence of annealing of each stacked layer on the growth and device performance is examined.

HL 6.7 Mon 11:00 EW 203

Atomic-scale structure of $Cu_2Zn(Sn,Ge)Se_4$ kesterite alloys — ●KONRAD RITTER¹, CORA PREISS¹, GALINA GURIEVA², RENÉ GUNDER², STEFANIE ECKNER¹, ROMAN CHERNIKOV³, EDMUND WELTER³, SUSAN SCHORR^{2,4}, and CLAUDIA S. SCHNOHR¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany — ³Deutsches Elektronen Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — ⁴Institut für Geologische Wissenschaften, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany

Kesterites offer a wide range of promising absorber materials for photovoltaics, but the record efficiency has not exceeded 12.6% yet. Alloying Sn with Ge or replacing it completely has been used in many different approaches in the literature. However, doing so might change the local structure of the material, which has been shown to influence macroscopic material properties such as the band gap energy. Extended X-ray Absorption Fine Structure Spectroscopy allows the local interatomic bond lengths to be probed and correlated with Ge content or off-stoichiometry of $Cu_2Zn(Sn,Ge)Se_4$ powder samples from solid state reactions. For the $Cu_2Zn(Sn,Ge)Se_4$ alloys it can be seen, that Ge uses the least space in the lattice and Sn the most. Furthermore, the nearest neighbour bond lengths do not change significantly with composition. This holds true for off-stoichiometric $Cu_2ZnGeSe_4$ samples as well.

15 min. break.

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Compositional inhomogeneity in kesterite thin film solar cell absorbers — ●MAURIZIO RITZER¹, SVEN SCHÖNHERR¹, PHILIPP SCHÖPPE¹, SERGIO GIRALDO², GERARDO LARRAMONA³, GALINA GURIEVA⁴, KONRAD RITTER¹, GEMA MARTÍNEZ-CRIADO⁵, SUSAN SCHORR^{4,6}, GILLES DENNLER³, EDGARDO SAUCEDO², CARSTEN RONNING¹, and CLAUDIA S. SCHNOHR¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany — ²Catalonia Institute for Energy Research, Spain — ³IMRA Europe S.A.S., France — ⁴Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — ⁵Instituto de Ciencia de Materiales de Madrid, Spain — ⁶Institut für Geologische Wissenschaften, Freie Universität Berlin, Germany

Kesterite $Cu_2ZnSnSe_4$ (CZTSe) is a promising absorber material for thin film solar cells. However, it often contains secondary phases that can limit their conversion efficiency. Moreover, the local kesterite composition may fluctuate on different length scales. High resolution, spatially resolved X-ray beam investigations enable insights into such compositional variations. Thin cross section lamellas were prepared out of complete solar cells using a focused ion beam system, in order to achieve high spatial resolution and to minimize averaging along the beam direction. Subsequently, the lamellas were scanned with the highly focused X-ray beam of 50 nm at the ID16B-NA station of the ESRF and by analyzing the emitted fluorescence (XRF) radiation we obtained elemental distribution maps. Thus, our approach easily allows to compare the composition within single grains and even grain boundaries.

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Identification of transparent p-type conducting non-oxide materials from high-throughput calculations — ●RAMYA KORMATH MADAM, THOMAS KÜHNE, and HOSSEIN MIRHOSSEINI — De-

partment of Chemistry, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

Transparent conducting materials (TCMs) have attracted attention owing to their diverse applications. Materials having wide band gap and low carrier effective mass have been considered as potential TCMs. Transparent conducting oxides (TCOs) have been largely commercialized as n-type TCMs in transistors, UV light emitting diodes, gas sensors, and tandem cells. However, the designing of efficient p-type TCOs are mainly hindered owing to the localized p character of their valence band which results in heavy holes. Hence, it is necessary to search for alternative potential p-type TCMs. In this work, high-throughput calculations were employed to determine the most promising p-type TCMs among chalcogenides. A large computational data set were investigated by data screening. Binary chalcogenides with band gaps > 1.7 eV and hole effective masses < 1 were considered for this study. Defect physics were investigated to probe the p-type performance of these semiconductors.

HL 6.10 Mon 12:00 EW 203

High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices — KORINA KUCHAR, ●MOHNISH PANDEY, KRISTIAN THYGESEN, and KARSTEN JACOBSEN — Technical University of Denmark (DTU), Lyngby - 2800, Denmark

We use computational screening to identify materials as light absorbers for photovoltaic (PV) and photoelectrochemical (PEC) devices. The screening is carried out on already synthesized compounds present in the ICSD database although yet unexplored for the PV and PEC applications. With thorough analyses of the properties like light absorption, charge carrier mobility, and defect tolerance we identify 74 materials including few already explored PV and PEC absorbers. Several recently investigated light absorbers such as $CsSnI_3$, $CsSnBr_3$, and $BaZrS_3$ also appear on the list.

HL 6.11 Mon 12:15 EW 203

Aluminum oxide passivation layers for $Cu(In,Ga)Se_2$ thin-film solar cells — ●FLORIAN WERNER¹, CONRAD SPINDLER¹, SUSANNE SIEBENTRITT¹, DIMITRI ZIELKE², and JAN SCHMIDT² — ¹Laboratory for Photovoltaics, Physics and Materials Science Research Unit, University of Luxembourg, L-4422 Belvaux, Luxembourg — ²Institute for Solar Energy Research Hamelin (ISFH), Am Ohrberg 1, D-31860 Emmertal, Germany

We employ ac and dc electrical measurements and photoluminescence to investigate the growth and passivation performance of aluminum oxide layers deposited by plasma-assisted atomic layer deposition (ALD) on $Cu(In,Ga)Se_2$. Already few monolayers of aluminum oxide hinder current flow through the device and result in non-linear current-voltage characteristics, which scale with the nominal thickness of the passivation layer. This indicates that a compact insulating layer is formed already after a few ALD cycles despite the larger surface roughness and different surface chemistry compared to standard single-crystalline silicon. Using plasma-assisted ALD, as-deposited aluminum oxide layers do not provide any meaningful surface passivation. Annealing for several minutes even at moderate temperatures of 350 °C results in a drastic improvement of the effective carrier lifetime, resulting in a level of surface passivation comparable to optimized CdS buffer layers. For such moderate annealing conditions we do not observe any indication of the formation of negative fixed charges, which would suppress interface recombination even further. A higher thermal budget, however, has so far led to a degradation of the passivated devices.

HL 6.12 Mon 12:30 EW 203

Insight into local fluctuations of net doping and lifetime in $Cu(In,Ga)Se_2$ solar cells — ●MAXIMILIAN KRAUSE¹, ALEKSANDRA NIKOLAEVA¹, JOSE MARQUEZ¹, CHARLES HAGES¹, SERGEJ LEVCENKO¹, THOMAS UNOLD¹, WOLFRAM WITTE², DIMITRIOS HARISKOS², and DANIEL ABU-RAS¹ — ¹Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Meitnerstr. 1, 70563 Stuttgart, Germany

It is known that local fluctuations in net doping and lifetime present in polycrystalline $Cu(In,Ga)Se_2$ (CIGS) thin films (with $\frac{[Ga]}{[In]+[Ga]} = 0.33$) can deteriorate the device performance of the corresponding solar cells via enhanced recombination. In order to investigate such fluctuations, electron-beam-induced current (EBIC) measurements were performed in a SEM on CIGS solar cells with different buffer lay-

ers: CdS, Zn(O,S), and In₂S₃ grown by chemical bath deposition. By fitting EBIC signals using appropriate models, the widths of the space-charge region, w_{SCR} , and also the diffusion lengths of the minority charge-carriers, L_{D} , were extracted. The order of magnitude of these values (400-500 nm and 1-2 μm) was verified by capacitance-voltage and quantum efficiency measurements. Although the values for w_{SCR} and therefore the average net doping of the CIGS layers were the same in the solar cells with the different buffer layers, substantial local variations of w_{SCR} were detected parallel to the p-n junction, which depend on the buffer/window stack applied. The present contribution discusses the impact of these fluctuations on the limitations of the device performance.

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Inhomogeneities in wide-gap Cu(In,Ga)Se₂ solar cells —
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Inhomogeneities in Cu(In,Ga)Se₂ solar cells related to the different net doping densities N_{A} in neighboring grains can limit the open-circuit voltage. The present work gives insight into local electrical and optoelectronic properties of wide-gap Cu(In,Ga)Se₂ solar cells ([Ga]/([In]+[Ga])=0.66) with different buffer layers by using electron-beam-induced current (EBIC) and cathodoluminescence measurements. Combining these techniques on the same identical position of cross-sectional specimens makes it possible to investigate the spatial distribution of inhomogeneities in the corresponding solar cells. From the EBIC profiles perpendicular to the substrate, values for the widths of the space-charge region w_{SCR} , which are proportional to $N_{\text{A}}^{-0.5}$, as well as for the diffusion lengths L_{D} of the charge carriers (related to the lifetime of the minority charge carriers) were extracted. It is shown that w_{SCR} and therefore N_{A} exhibits fluctuations depending on the buffer layer applied. The average values of w_{SCR} and L_{D} were confirmed by capacitance-voltage and quantum efficiency analysis of the solar cells.