

HL 4: Focused Session: Inhomogeneous Materials for Solar Cells I

Although multinary compound semiconductors exhibit a variety of inhomogeneities - such as strong local concentration fluctuations, built-in vertical concentration gradients, rough interfaces, and a high density of grain boundaries - they are among the leading solar cell technologies. In this focused session, the impact of inhomogeneities on the carrier transport in solar cells shall be addressed with emphasis on material growth, characterization, and modeling. Therefore, state-of-the-art research and challenges will be highlighted for a broad range of related materials such as chalcopyrites, kesterites, perovskites, and group III-nitrides.

Organizers: Roland Scheer (MLU Halle Wittenberg), Frank Bertram (OvGU Magdeburg), and Jürgen Christen (OvGU Magdeburg)

Time: Monday 9:30–12:15

Location: CHE 89

Topical Talk HL 4.1 Mon 9:30 CHE 89

Inhomogeneities in chalcopyrites and kesterites — ●CLAUDIA S. SCHNOHR — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Thin film solar cells based on Cu(In,Ga)(Se,S)₂ have reached a record efficiency of 22.6%, thus closing the gap to silicon-based technology. Cu₂ZnSn(Se,S)₄ has also attracted great attention as non-toxic, earth-abundant alternative and a record efficiency of 12.6% has already been demonstrated. Both material systems typically feature inhomogeneities such as grain boundaries, interfaces, and compositional variations, that may deteriorate or improve the device performance. We therefore applied high-resolution X-ray fluorescence analysis using a synchrotron nanobeam to study the elemental composition of chalcopyrite- and kesterite-type thin films on a micrometer and submicrometer scale. To that end, thin cross section lamellas were prepared with a focused ion beam system. For Cu(In,Ga)(Se,S)₂, the depth-dependent Ga gradient shows a strong dependence on the growth conditions in a sequential two-stage process. Furthermore, we find subtle lateral variations in the material composition and a significant In enrichment for some of the grain boundaries. For highly non-stoichiometric Cu₂ZnSn(Se,S)₄, different binary secondary phases coexist within a distance of only a few micrometers and the local compositions of the kesterite-type domains differ tremendously from the integral layer composition. Detailed knowledge of these compositional variations, which directly affect the electronic properties of the material, will thus help to exploit the full potential of chalcopyrite- and kesterite-based thin film solar cells.

Topical Talk HL 4.2 Mon 10:00 CHE 89

Impact of growth condition on defect generation in Cu(In,Ga)Se₂ — ●TAKEAKI SAKURAI¹, MUHAMMAD ISLAM¹, AKIRA UEDONO¹, SHOGO ISHIZUKA², HAJIME SHIBATA², SHIGERU NIKI², and KATSUHIRO AKIMOTO¹ — ¹University of Tsukuba, Tsukuba, Japan — ²National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

Characterization of defects in Cu(In,Ga)Se₂ (CIGS)-based solar cells is an important research subject for understanding its carrier recombination processes. In this decade, the optical and electrical response of the defect states have been intensely studied using various analytical methods. Nevertheless, the origin and distribution of the defects in CIGS have not been fully understood yet due to its complex device structures and multinary compositions. During the growth of CIGS, in particular, segregation of the secondary phase, selenization, and alkali metal diffusion occur, and the difficulty in the control of the growth process mainly results in fluctuation of their optoelectronic properties. Therefore, a systematic study on the relation between the thin film growth and the generation of defects is necessary. In this study, we have investigated the impact of growth condition (Se flux and Ga concentration) on defect generation in CIGS by using various characterization techniques. We want to point out that the defect level centered around 0.8 eV from the valence level may act as a recombination center at room temperature. We will discuss whether this defect level acts as a recombination center by using two-wavelength excited photoluminescence method.

HL 4.3 Mon 10:30 CHE 89

On the impact of material inhomogeneities on the time-resolved luminescence decay — ●MATTHIAS MAIBERG, TORSTEN HÖLSCHER, and ROLAND SCHEER — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany

Time-resolved luminescence is the method of choice for determination of material parameters, e.g. the minority carrier lifetime in a semiconductor. However, due to the size of the excited area the obtained data are mostly mean values averaged over a typical region of 10⁴ cm⁻². In our work, we study the impact of lifetime fluctuations, band gap inhomogeneities, and potential fluctuations on the time-resolved luminescence decay by means of three-dimensional simulation. It turns out that inhomogeneous charge carrier lifetimes will increase the luminescence decay time, if the ratio of the structure size and the average diffusion length is larger than 1. For ratios smaller than 1, however, inhomogeneous charge carrier lifetimes will lead to reduced luminescence decay times. In contrast to the strong impact of lifetime inhomogeneities, band gap fluctuations are shown to have a negligible effect on the luminescence decay. In the end, it is demonstrated that the effect of potential fluctuations, which numerous of the thin-film semiconductors are prone to, is rather similar to that of space charges in a semiconductor junction. In particular the decay time will always be smaller than the recombination lifetime due to occurring drift effects. For this reason, potential fluctuations may not explain the often observed long decay times in compensated semiconductors such as Cu(In,Ga)Se₂ or Cu₂ZnSnSe₄.

15 min. break.

Topical Talk HL 4.4 Mon 11:00 CHE 89

Inhomogeneities in chalcopyrites for solar cells — ●DANIEL ABOU-RAS — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Thin-film solar cells with polycrystalline Cu(In,Ga)(S,Se)₂ absorber layers have exhibited record conversion efficiencies of up to 22.6%. Although parallel to the substrate, the concentrations of the matrix elements in these Cu(In,Ga)(S,Se)₂ thin films do not vary substantially, obvious inhomogeneities are the [In]/[Ga] and also (in case S is present) [S]/[Se] gradients perpendicular to the substrate. Moreover, also indications for various net doping concentrations in neighboring grains have been reported, which may be explained by locally varying point-defect concentrations. On the (sub)nanometer scale, compositional variations at different line and planar defects in Cu(In,Ga)(S,Se)₂ thin films have been detected. The present contribution will give an overview of all these inhomogeneities existing on different length scales, but all affecting the potential landscape of chalcopyrite-type Cu(In,Ga)(S,Se)₂ absorber layers.

Topical Talk HL 4.5 Mon 11:30 CHE 89

Understanding the defects in Cu(In,Ga)Se₂ solar cell: a correlative microscopy approach — ●OANA COJOCARU-MIRÉDIN¹, TORSTEN SCHWARZ², ROLAND MAINZ³, and DANIEL ABOU-RAS³ — ¹University of RWTH Aachen, I. Institut of Physics, Sommerfeldstraße 14, 52056 Aachen, Germany — ²Max-Planck Institut für Eisenforschng, Max-Planck Straße 1, 40237 Düsseldorf, Germany — ³Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany

In Cu(In,Ga)Se₂ solar cells, interfaces between individual layers in a thin-film stack, such as p-n heterojunctions, or structural defects such as grain boundaries or stacking faults, often influence substantially the performance of the device [1]. To further develop these solar devices, one needs to understand the relationship between structural and chemical properties for specific interfaces and defects. Diffraction techniques in transmission electron microscopy or scanning electron microscopy are excellent tools for structural investigations, i.e., the

crystallographic structure of stacking faults and grain boundary. The present work shows an advanced, correlative study combining atom-probe tomography and various electron microscopy techniques on defects in Cu(In,Ga)Se₂ absorber. Indeed, different approaches for determining structural and chemical property relationships will be presented. The experimental results to be presented will also be compared directly with the existing theoretical models on defects and phase formation in photovoltaic materials.

[1] M. Müller et al., Journal of Applied Physics 115 (2014) 023514.

HL 4.6 Mon 12:00 CHE 89

Controllable crystallization of chalcogenide thin films for photovoltaic and electrical applications — •ILIA KOROLKOV, MICHEL CATHELINAUD, XIAN-HUA ZHANG, and JEAN-LUC ADAM — Verres et céramique, ISCR, Université de Rennes 1, Rennes, France

Chalcogenide materials (i.e. materials containing sulfur (S), selenium (Se) and/or tellurium (Te)) are of great importance in the context

of solar energy harvesting because of their suitable electronic properties such as extended absorption spectrum, direct band gap and high absorption coefficient.

In this work we present the investigation on chalcogenide thin films of 40Sb₂Se₃-40GeSe₂-20CuI composition, which upon the crystallization showed the formation of the conductive percolation network formed by Sb₂Se₃ rods covered with Cu₂GeSe₃ microcrystals. We optimized targets composition varying the amount of iodine and copper iodide. Various deposit and heating treatment regimes were applied as well. We revealed an important role of the iodine which dopes Sb₂Se₃, increasing drastically its conductivity and serving as an electron donor. We established that pre-deposit of a very thin film of CuI (about 3nm) prior to a major thin film deposit influences positively on crystallization and conductive channels formation during the heating treatment. A simple photovoltaic cell of [ITO|ZnO (or Sb₂Se₃ : I)|40Sb₂Se₃-40GeSe₂-20CuI|Au] configuration shows the short circuit current up to 10mA/cm² and open circuit voltage up to 0,2V.