MM 31: Topical Session Photovoltaic Materials II

Time: Wednesday 11:45–13:15 Location: H4

MM 31.1 Wed 11:45 H4

The influence of reducing the chalcogen to metal ratio on phase transitions during the crystallisation of photovoltaic materials CuIn(S,Se)2 — •Astrid Hölzing[1], Roland Schurr[1], Stefan Jost[2], Jörg Palm[2], Barbara Tautz[3], Felix Oehlschläger[3], Ulrike Künecke[3], Klaus Deseler[3], Peter Wellmann[3], and Rainer Hock[1] — [1]Lehrstuhl für Kristallographie und Strukturphysik, FAU, Erlangen, Deutschland — [2]Avancis GmbH & Co. KG, München, Deutschland — [3]Materials for Electronics and Energy Technology, FAU, Erlangen, Deutschland

Time resolved monitoring of the crystallisation of the thin film absorber materials CuIn(S,Se)2 while annealing stacked elemental layers (SEL) yields phase transitions proceeding during the chalcopyrite synthesis. In-situ XRD and DSC measurements on similar processed precursors provide complementary information on intermediate phases and the reaction kinetics of the chalcopyrite formation can be obtained. Thin layers of metals and chalcogens are deposited onto Mo-coated substrates by DC-magnetron sputtering and thermal evaporation, respectively. The XRD powder diagrams recorded while annealing the SEL are quantitatively analysed by Rietveld refinements. Miscellaneous binary selenides and sulfides as well as ternary sulfoselenides are observed by the chalcogenisation of the intermetallic alloy yielding different educts for the chalcopyrite formation depending on the chalcogen content. The presented study will be focused on the influence of reducing the chalcogen to metal ratio on the processing of photovoltaic materials CuIn(S,Se)2.

MM 31.2 Wed 12:00 H4

Properties of grain boundaries in Cu(In,Ga)Se$_2$ and Cu(In,Ga)S$_2$ thin film solar cells deduced from mean inner coulomb potential measurements — •Sebastian S. Schmidt[1], Daniel Abou-Ras[1], Joachim Klaer[1], Raquel Caballero[1], Christoph T. Koch[2], Thomas Unold[1], and Hans-Werner Schock[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Max Planck Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Polycrystalline Cu(In,Ga)Se$_2$ and Cu(In,Ga)S$_2$ thin films are efficient absorbers in thin film solar cells. The solar cell efficiencies strongly depend on the physical properties of grain boundaries in the absorbers. Here, we investigate the local behavior of the mean inner coulomb potential (MIP) at grain boundaries in Cu(In,Ga)Se$_2$ and Cu(In,Ga)S$_2$ solar cell absorbers. With in-line holography in a transmission electron microscope we measure MIP wells at grain boundaries in both types of absorber layers. The depth of the MIP wells depends on the grain boundary type as well as the composition. Generally, the potential wells have a FWHM of about 1 nm perpendicular to the plane of the grain boundary. Since the Debye length is about 10-40 nm in the absorber layers, considerable excess charge accumulations and related band bending at the analyzed grain boundaries can be excluded. A variation in composition seems to be responsible for the formation of MIP wells at grain boundaries. We discuss the local composition at grain boundaries by utilizing the isolated atom approximation.

MM 31.3 Wed 12:15 H4

Structural and chemical analyses of MOVPE-grown CuGaSe$_2$ layers on (001)-GaAs — •Stefanie Bierwirth[1], Susanne Siebentritt[2], Levent Gütay[2], Jes Larsen[2], and Michael Seibt[1] — [1]Universität Göttingen — [2]Université du Luxembourg

This contribution has been withdrawn.

MM 31.4 Wed 12:30 H4

Characterisation of thin C60 films using X-Ray methods — •Chris Elschner, Alexandr A. Levin, Christoph Schuenemann, Moritz Riede, and Karl Leo — TU Dresden, Institut für Angewandte Photophysik 01069 Dresden George-Bähr-Straße 1

C60 is a well known and often used molecule for state of the art organic solar cells. To increase the efficiency in these nanoscale systems, it is necessary to control the morphology of the thin film layers with the aim to optimize the electrooptical properties. Thin C60 film layers are produced via vacuum deposition under variation of substrate temperature from 30°C up to 90°C, film thickness from 25 nm to 50 nm, and vacuum chamber pressure. The characterisation of the film layers is carried out using x-ray reflection (XRR) and x-ray diffraction (XRD). From these results, the crystallinity, the film thickness, the roughness, and the density of the film layer can be estimated. Using the Scherrer equation, we estimate the average crystal size, which shows the existence of nanoscale crystals (10 nm) in a 50nm C60 film. These results are the base for the coming investigations of mixed organic layers for the use in organic solar cells.

MM 31.5 Wed 12:45 H4

Effect of film thickness, type of buffer layer, and substrate temperature on the morphology of dicyanovinyl-substituted sexithiophene films — •Alexandr A. Levin[1], Marieta Levichkova[1], Martin Pfeiffer[2], Dirk Hildebrandt[2], David Wynands[1], Chris Elschner[1], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Heliatek GmbH, 01187 Dresden, Germany

Dicyanovinyl-substituted sexithiophenes (DCV6T) are promising photoactive materials [1]. The influence of the film thickness, type of buffer underlayer, and deposition substrate temperature on the morphology of the DCV6T layers is investigated by means of X-ray diffraction and X-ray reflectivity methods. A neat Si wafer or a Si wafer covered by a 15 nm buffer underlayer of fullerene C60 or 9,9-Bis[4-(N,N-bis-biphenyl-4-yl-amino)phenyl]-9H-fluorene (BPAPF) is used as substrate.

The crystalline nature and ordered molecular arrangement of the films are proven down to 6 nm film thickness. With increasing substrate temperature or film thickness, the DCV6T film relaxes, resulting in reducing the interplane distances (from 11.29(5) Å to 10.78(5) Å) closer to the bulk value (10.14(1) Å). Considering the same thickness, the DCV6T film relaxes for growth on Si to BPAPF to C60. Thicker films are characterized by smaller density and higher roughness. A thin (some nm-thick) intermediate layer with linear density-gradient is formed in DCV6T/C60 interface for the films with buffer C60 layer.

[1] D. Wynands et al., J. Appl. Phys. 106 (2009) 054509.

MM 31.6 Wed 13:00 H4

Morphological study of Zinc-Phthalocyanine for organic solar cells — •Christoph Schünemann, Chris Elschner, Alexandr Levin, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Germany

Phthalocyanines (Pc) are well known organic molecules and often used in the photoactive layer of small molecule organic solar cells. Reasons for the wide application of these organic semiconductors are their thermal stability, simple way of deposition and their common use as model system. However, the influence of the morphology on the electrical properties of organic solar cells has been investigated only rudimentary so far. In this work, the crystal structure, the growth and the stacking of Zinc-Pc molecules in thin films are investigated with x-ray diffraction (XRD) and x-ray reflection (XRR) methods. For this purpose, we varied the ZnPc film thickness from 5 nm up to 50 nm and the substrate temperature while deposition from room temperature up to 90 °C. Using XRR and atomic force microscopy, we found that the roughness of ZnPc increases with increasing substrate temperature and layer thickness. The XRD measurements show that the ZnPc layers are polycrystalline for all substrate temperatures and layer thickness. Analysing the XRD pattern we also found out, that the ZnPc films are triclinic and the atomic structure does not change with variation of the deposition parameters. The dislocation density and the microstrain in the ZnPc layer decreases with rising film thickness while the crystallite size is in the range of the layer thickness.