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The interplay between off-stoichiometry and intrinsic point defects in quaternary compound semiconductors

Thin film photovoltaic is an emerging alternative technology because of short energy payback time and minimum use of high purity materials, addressing the urgent need for cost-competitive renewable energy technologies. Compound semiconductors, like chalcopyrite type $Cu(In,Ga)(Se,S)_2$ (CIGSe), are the most advanced and most efficient absorber materials. Such solar cells show present record lab efficiencies of >22%. Since the availability of indium is an object of concern regarding the large scale production of solar cells, its replacement with Zn and Sn is beneficial in this sense. Compounds like $Cu_2ZnSn(S,Se)_4$ (CZTS, CZTSe) are an alternative. One of the reasons for the success of CIGSe based thin film solar cells is the remarkable flexibility of its chalcopyrite type crystal structure. This flexibility is a key also for the quaternary kesterite type compounds CZTS, Se because the thin film growth is in fact a non-equilibrium process. The absorber layers of high efficient solar cells exhibits an overall off-stoichiometric composition, thus the existence of intrinsic point defects is strongly correlated with the chemical potential and therefore dependent on the composition of the material. These structural defects influence the electronic properties of the final device sensitively. A high density of bulk defects and structural disorder (Cu/Zn disorder) will cause extreme band tailing which could account for a significant part of the V_{oc} loss, the main limitation for the performance of CZTS, Se-based PV devices. Our research focuses on the correlation between off-stoichiometry, point defects and physical properties of kesterites. We have demonstrated that kesterite type CZTSe can self-adapt to Cu-poor and Cu-rich compositions without any structural change except the cation distribution. The ability to accept deviations from stoichiometry, which can be categorized in off-stoichiometry types (A-L), is correlated to a Cu/Zn disorder and the formation of intrinsic point defects (see fig. 1).

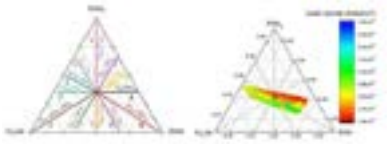

Figure 1: Off-stoichiometry types A-L (left) and Cu/Zn disorder (right) in dependence on stoichiometry deviations in CZTSe. The point in the middle of the ternary phase diagram marks CZTSe, the dotted lines correspond to the off-stoichiometry types shown left.

On the other hand, Cu/Zn disorder correlates with physical properties, like a shift of the hotoluminescence (PL) peak position. Hence we were able to show quantitatively that Cu/Zn disorder in kesterites causes shifts in the energy band gap giving raise to band tailing.

Biography

Susan Schorr has obtained her PhD in physics from the Technical University Berlin in 1995. She was Postdoc in the inelastic neutron scattering group at the Hahn-Meitner-Institute Berlin and Visiting Scientist at the Los Alamos National Laboratory, US. She started as a Research Associate at the University Leipzig where she finished her Habilitation in 2006. At this time she started to work on multinary compound semiconductors for PV applications and developed the average neutron scattering length analysis method to evaluate the materials intrinsic point defects. She went back to the Hahn-Meitner-Institute Berlin (now HZB) to join the Institute of Technology in the Solar Energy Division as a Group Leader. In 2008, she was appointed as Professor for Geo-Materials Research at the Freie Universitat Berlin and became Head of the Department Structure and Dynamics of Energy Materials at the Helmholtz-Zentrum Berlin for Materials and Energy (HZB).

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