Modelling of Extended Defects in CIGS Based Solar Cells

Researchers
Daniel Barragan-Yani

Principal Investigator
Prof. Dr. rer. nat. Karsten Albe

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Project Areas
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Clusters
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Institute
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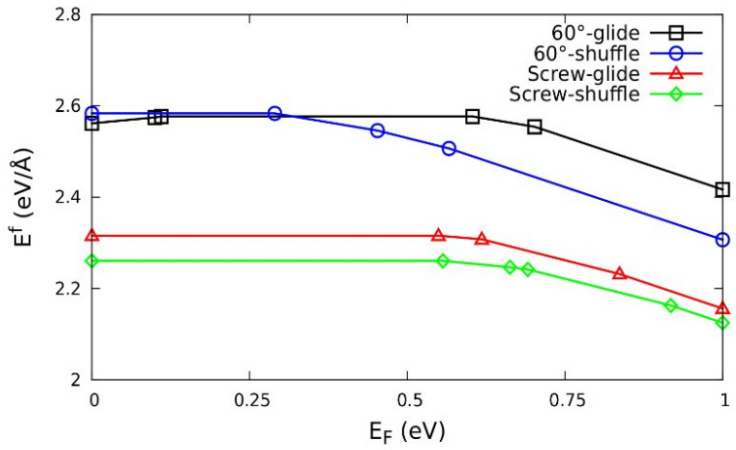
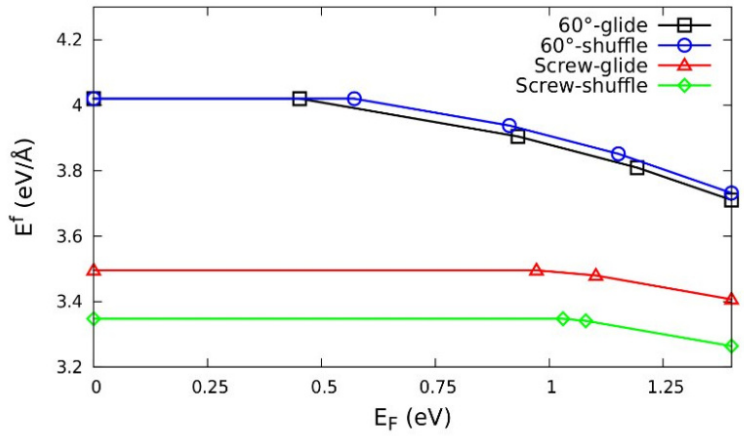


a)



b)

Fig. 1: These results are a first and relevant step towards understanding the apparent harmless nature of dislocations in the Cu(In,Ga)Se_2 based solar cells.

Introduction

Chalcopyrite Cu(In,Ga)Se2 (CIGSe) are one of the most succesful materials used as absorber layer in thin-film solar cells[1,2]. The optical and electronic properties of these compounds can be tunned with Ga-In ratio and depend strongly on the presence of defects. Point defects and their properties have been studied extensively [3,4]. One further type of defect that has captured a great deal of attention are grain boundaries. Their properties are interesting since polycristalline CIGS-based solar cells overcome their crystalline counterparts[5,6]. In spite of substantial research efforts, a complete understanding of the physics behind the influence grain boundaries have on the device performace is still lacking. Besides grain boundaries, other extended defects have been identified. This includes twin boundaries, stacking faults and dislocations. However, no much theoretical research has been conducted in order to clarify the role played by dislocations in CIGS even when their presence is undeniable. By means of transmission electron microscopy, high dislocation densities up to 10^10 -10^11 cm^−2 were found in solar cells with power-conversion efficiencies up to more than 15% [7]. Contrary to what is found in poly-crystalline silicon[8,9], the fact that decent efficiencies are reached with such high presence of dislocations is a remarkable property and is necessary to answer wich electrical properties of dislocations in CIGSe layers allow for such behavior.

Methods

The resources appointed in the Lichtenberg cluster have been used to study the structural parameters, electronic structure and formation energies of the relaxed glide and shuffle dislocation cores with smallest Burgers vectors (b) in a chalcopyrite structure, the screw and the 60° types. To achieve such goal we have used density functional theory (DFT) and a Hubbard corrected local density approximation (LDA+U)[10] approach as implemented in the Vienna Ab-Initio Simulation Package VASP[11].

Results

The results obtained show that in both CuInSe_2 and CuGaSe_2, the ternary parent compounds of CIGSe, screw dislocations present distorted bonds but the atoms configurations after relaxation are such that full coordination is maintained. On the other hand, relaxed structures of the 60◦ mixed dislocations do not show reconstruction and dangling bonds are patent. As expected, DOS of the relaxed core structures show shallow defect states for all structures under study and two deep defect states for the glide 60◦ dislocation. The defect states were further studied by means of the charge density associated with them. A clear feature observed for all states was localization in the volume surrounding the cores.

Finally, the calculated core formation energies, figure 1, show that for the positive doping regime (p-type), only the glide 60° dislocations in CuInSe_2 prefer a positively charged state. For

the same regime and in the most relevant region of it, all the other dislocation types studied here are charge neutral and therefore, electrically inactive.

Reference

[1] I. Repins, M.A. Contreras, B. Egaas et al. (2008): 19·9%-efficient ZnO/CdS/CuInGaSe2 solar cell with 81·2% fill factor. Progress in Photovoltaics: Research and Applications 16, 235. https://doi.org/10.1002/pip.822

[2] P. Jackson, D. Hariskos, E. Lotter et al. (2011): New world record efficiency for Cu(In,Ga)Se2 thin-film solar cells beyond 20%.Progress in Photovoltaics: Research and Applications 19, 894. https://doi.org/10.1002/pip.1078

[3] S. B. Zhang, S.-H. Wei, A. Zunger, and H. Katayama-Yoshida (1998): Defect physics of the CuInSe2 chalcopyrite semiconductor. Phys. Rev. B 57, 9642. https://doi.org/10.1103/PhysRevB.57.9642

[4] J. Pohl and K. Albe (2013): Intrinsic point defects in CuInSe2 and CuGaSe2 as seen via screened-exchange hybrid density functional theory. Phys. Rev. B 87, 245203. https://doi.org/10.1103/PhysRevB.87.245203

[5] C. Persson and A. Zunger (2003): Anomalous Grain Boundary Physics in Polycrystalline CuInSe2: The Existence of a Hole Barrier. Phys. Rev. Lett. 91, 266401. https://doi.org/10.1103/PhysRevLett.91.266401

[6] S. S. Schmidt, D. Abou-Ras, S. Sadewasser et al. (2012): Electrostatic Potentials at Cu(In,Ga)Se2 Grain Boundaries: Experiment and Simulations. Phys. Rev. Lett. 109, 095506. https://doi.org/10.1103/PhysRevLett.109.095506

[7] J. Dietrich, D. Abou-Ras, S.S. Schmidt et al. (2014): Origins of electrostatic potential wells at dislocations in polycrystalline Cu(In,Ga)Se2 thin films. Journal of Applied Physics 115,103507. https://doi.org/10.1063/1.4867398

[8] C. Donolato (1998): Modeling the effect of dislocations on the minority carrier diffusion length of a semiconductor. Journal of Applied Physics 84. https://doi.org/10.1063/1.368378

[9] T. Kieliba, S. Riepe, and W. Warta (2006): Effect of dislocations on minority carrier diffusion length in practical silicon solar cells. Journal of Applied Physics 100, 093708. https://doi.org/10.1063/1.2338126

[10] S.L. Dudarev, G.A. Botton, S.Y. Savrasov, C.J. Humphreys, and A. P. Sutton (1998): Electron-energy-loss spectra and the structural stability of nickel oxide: An LSDA+U study. Phys. Rev. B 57, 1505. https://doi.org/10.1103/PhysRevB.57.1505

[11] G. Kresse and J. Furthmüller (1996): Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Phys. Rev. B 54, 11169. https://doi.org/10.1103/PhysRevB.54.11169

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