11A/B,12001G331

The Chemical Environment about Cd atoms in Cd Chemical Bath Treated $CuInSe_2$

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Introduction

CdS buffer layers located between the p-type $Cu(In;Ga)Se_2$ (CIGS) absorber layer and the n-type ZnO window layer have become an integral part of high-efficiency polycrystalline CIGS solar cells. Experimentally it has been found that the highest conversion efficiencies occur in cells with chemical-bath deposited (CBD) CdS buffers. Even though the amount of Cd incorporated into the cells is minute, an effort has been made to understand the reasons for the efficacy of the CDB-CdS buffer as a preamble to find alternative, less toxic substitutes. Several recent reports have concluded that treatment by (partial electrolyte) PE-Cd alone, or in combination with conventional CBD-CdS deposition results in improvement in either cell performance or reproducibility[1]. An outstanding question that must be answered before detailed investigation of the underlying mechanism can begin is where in the CIGS matrix the CBD deposited Cd resides. We have used near-edge x-ray absorption fine structure (XANES) at the Cd-L_3 edge (3537 eV) to selectively investigate the local atomic environment about Cd atoms in CBD-Cd treated polycrystalline $CuInSe_2$ and $CuGaSe_2$ deposited on Mo-coated soda-lime glass substrates which were then compared with first-principles calculations.

Experiment

Both the $CuInSe_2$ and $CuGaSe_2$ samples used in this study were deposited by the three-stage method onto Mo-coated soda-lime glass substrates.[2] The as-grown samples were placed into a CBD-Cd chemical bath kept at a temperature of 40° for 40 minutes. The Cd precursor used was CdI_2 (0.7×10^{-3} mol/l) in an NH_4OH 0.5 mol/l solution. After deposition, the samples were then introduced into a vacuum chamber at beam line BL11B at the Photon Factory in Tsukuba, Japan. The Cd-L_3 edge (3537 eV) was excited in glancing incidence mode and fluorescence data was taken using a windowless Ge SSD.

Results and Discussion

Fig. 1 show both experimental data for the Cd-L_3 edge taken for both $CuInSe_2$ and $CuGaSe_2$ CBD-Cd treated films in fluorescence mode. In addition to the experimental data the results of theoretical calculations done using the *ab initio* code feff 8.10[3] are shown for Cd residing in different places in the host matrix as well as Cd in metallic and oxide form. The feff calculations were performed using a self-consistent field approach as well as full multiple scattering on a cluster of radius 0.8 nm.

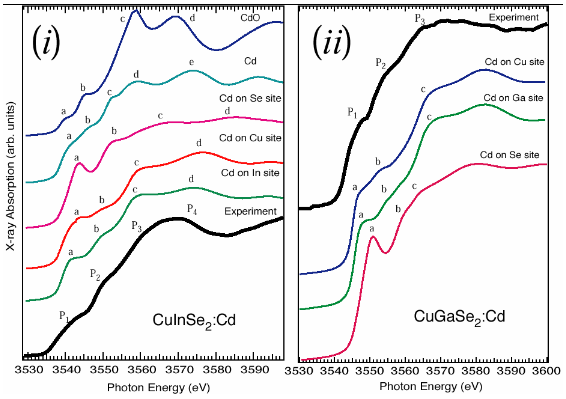

Figure 1: Experimental and simulated Cd-L_3 XANES spectra for CBD-Cd treated $CuInSe_2$ (*i*) and $CuGaSe_2$ (*ii*) films

Conclusion

We have measured the local structural environment of Cd in CBD-Cd treated $CuInSe_2$ and $CuGaSe_2$ polycrystalline samples using XANES at the Cd-L_3 edge and compared the experimental results to theoretical simulations. Similar results were found for both materials, namely that Cd most likely resides on the cation sites alone. The current experiments cannot distinguish between which of two cation sites the Cd ions reside upon. The presence of Cd on both cation sites also implies the near surface layer may be strongly electrically compensated.

References

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