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Understanding the structural disorder of (AgxCu1-x)2ZnSnSe4 based Kesterite semiconductor by neutron diffraction study.

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The quaternary semiconductor Cu2ZnSnSe4 (CZTSe) is a promising environment-friendly and low-cost material as a solar cell absorber layer with a power conversion efficiency of 11.6%. Its photovoltaic performance is currently limited due to its disorder between the Copper & Zinc lattice sites, which creates band tailing and creates voltage deficit. By replacing Cu in CZTSe with isovalent Ag, whose ionic radius is larger than that of Cu and Zn, the density of I–II antisite defects could be suppressed. This work has been done to quantify the cation disorders on all cation symmetry sites and the effect of substitution of Ag in the CZTSe crystal structure. (AgxCu1-x)2ZnSnSe4 (A/CZTSe) samples with different compositions were synthesized by a solid-state reaction of the pure element in an evacuated quartz tube. Structural analysis of stoichiometric & off-stoichiometric samples were performed using Raman and synchrotron powder diffraction including Rietveld refinement. A neutron diffraction experiment is performed to fully understand the cation distribution analysis in A/CZTSe powder sample as Cu+ and Zn2+ are not distinguishable using conventional X-ray diffraction method due to their isoelectronic character but there is a significant difference in their neutron scattering length (bCu = 7.718 fm, bZn = 5.680 fm). It is found that powder A/CZTSe adopts the kesterite type structure with a partial disorder of copper and zinc on the two Wyckoff position 2c and 2d. Sn has been found on Wyckoff position 2b (0, 0, ½), whereas Cu/Zn is located on 2a (0, 0, 0), 2c (0, ½ , 1/4) and 2d (0, ½ , ¾) sites. There is a presence of copper vacancies (VCu), various cation anti-site defects (CuZn, ZnCu, ZnSn, and SnZn) have been found for different compositions. This work will also answer the effectiveness of Ag as a substitution of Cu in kesterite based CZTSe, to suppress anti-site disorder.

Speakers Gender

Female

Level of Expertise

Student

Do you wish to take part in the poster slam

Yes

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