



Contribution ID: 105

Type: **Poster contribution**

Cu/Zn disorder in $\text{Cu}_2\text{ZnSn}(\text{S}_x\text{Se}_{1-x})_4$ monograins: the result of “ordering” procedure

Kesterite-type based thin film solar cell technologies are mainly based on polycrystalline absorber layers. A promising low cost alternative technology uses $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ (CZTSSe) monograins (single crystals of 50-100 μm size) which are fixed in a polymer matrix to form a flexible solar cell [1].

It is agreed in literature that large band tailing observed in Cu-based kesterite-type semiconductors causes voltage losses limiting the efficiency of kesterite-based devices. The Cu/Zn disorder (CuZn and ZnCu anti-sites in Cu-Zn planes at $z=\frac{1}{4}$ and $\frac{3}{4}$), which is always present in these compounds [2], is discussed as a possible reason for band tailing.

The experimental determination of the order parameter Q which is a quantitative measure of the degree of Cu/Zn disorder [3] requires a differentiation between the isoelectronic cations Cu^+ and Zn^{2+} . An in depth analysis of neutron diffraction data provides information on the cation distribution in the crystal structure allowing the determination of type and concentration of intrinsic point defects including a distinction between Cu and Zn [2]. On the other hand neutron diffraction requires large sample volumes, thus kesterite monograins offer the unique possibility to correlate structural disorder in kesterite-type absorbers with device performance parameters.

We will present a detailed structural investigation of the effect of the disordering procedure and the long low temperature – “ordering” annealing on the Cu/Zn disorder and optical properties of the CZTSSe monograins will be presented.

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Session Classification: Energy materials: batteries, photovoltaics, etc.

Track Classification: Energy materials: batteries, photovoltaics, etc.