**Poster Presentation**

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## *Cation disorder in CZTS materials from anomalous diffraction at KMC-2 (BESSY)*

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The compound semiconductor Cu2ZnSnS4 (CZTS) is a promising alternative for absorber layers in thin film solar cells, as it has a nearly ideal band gap of about 1.5 eV, a high absorption coefficient for visible light, and contains only earth abundant and non-toxic elements. Besides chemical composition and phase purity, the efficiency of CZTS thin film solar cells depends strongly on the concentration of Cu- and Zn-antisites and copper vacancies in the kesterite-type structure. However, Cu(I) and Zn(II) are isoelectric and thus cannot be distinguished by conventional X-ray diffraction. In prior work we determined Cu-Zn-distribution successfully from neutron scattering [1]. Here we present experiments utilizing anomalous X-ray diffraction on the K-edges of Cu and Zn. Anomalous scattering coefficients are heavily wavelength-dependent close to the absorption edges of the respective element. This is utilized for contrast enhancement. Usage of multiple wavelengths above, below and between the absorption edges of Cu and Zn ensures significant overdetermination, so that the Cu-, Zn-, and vacancy concentrations can be refined reliably for the independent crystallographic sites. Experiments were conducted at the diffraction end station of the KMC-2 beamline [2] at BESSY (Berlin, Germany). KMC-2 provides X-ray radiation with both very stable energies and intensities. The accessible energy range of 4 – 14 keV is ideally suited for the K-edges of Cu (8979 eV) and Zn (9659 eV). A 6-circle goniometer in psi-geometry allows both powder and grazing incidence diffraction, so that bulk samples and thin films can be measured. The instrument can be equipped with either a scintillation point detector (Cyberstar) or an area detector (Bruker Vantec), allowing to optimize resolution and intensity to the needs of the experiment.

***[1]*** *S. Schorr, Sol. Energy Mat. and Sol. Cells. 2011, 95, 1482-1488,* ***[2]*** *A. Erko, I. Packe, C. Hellwig et al., AIP Conference Proceedings 2000, 521, 415-418*

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