MS16-05 | MEAD, SALT, AND SUNSHINE: CATION DISTRIBUTION IN CZTSE, CFTS, AND CZSISE

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Multiple Edge Anomalous Diffraction (MEAD) [1] has been applied to various quaternary sulfosalts belonging to the adamantine compound family in order to validate the distribution of copper, zink, and iron cations in the structure. Semiconductors from this group of materials are promising candidates for photovoltaic applications. Their properties are strongly depended on point defects, in particular related to cation order-disorder. However, Cu^{+1}, Zn^{2+}, and Fe^{2+} have very similar scattering factors and are all but undistinguishable by normal X-ray diffraction. Anomalous diffraction utilizes the dependency of the atomic scattering factors *f'* and *f''* from the energy of the radiation, especially close to the element-specific absorption edges. In the technique called MEAD individual Bragg peaks are tracked over an absorption edge. The intensity changes depending on the structure factor can be highly characteristic for Miller indices selected for a specific structural problem, but require very exact measurements. Beamline KMC-2 [2] at synchrotron BESSY II, Berlin has been recently upgraded for this technique. Anomalous X-ray powder diffraction and EXAFS compliment the data.

[1] B. A. Collins *et al*.: *Physical Review B* **92**, 224108 (2015)
[2] Helmholtz-Zentrum Berlin für Materialien und Energie: *J large-scale research facilities*, **2**, A49 (2016)