Poster

Deep insights into energy materials utilizing anomalous X-ray diffraction

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Cation arrangement, disorder and defects substantially impact the optoelectronic properties of multinary semiconductors [1]. While often an inconvenience, this also provides opportunities to enhance optical properties such that improved absorption coefficient and photovoltaic device efficiency can be achieved [1]. Due to the fundamental relationship between atomic geometry, electronic structure and physical properties such tuning requires a solid knowledge of the atomistic material structure.

Isoelectric cations are hard to distinguish by laboratory X-ray diffraction. Besides neutron radiation, anomalous X-ray diffraction is commonly used to overcome this problem, utilizing the strong energy dependency of scattering factors close to the element-specific X-ray absorption edges. A variant of this, Multiple Edge Anomalous Diffraction (MEAD) [2] was found by us to work particularly well for determination of cation arrangements within a known parent structure. This method calls for measuring the energy dependency of the intensity of selected individual Bragg peaks.

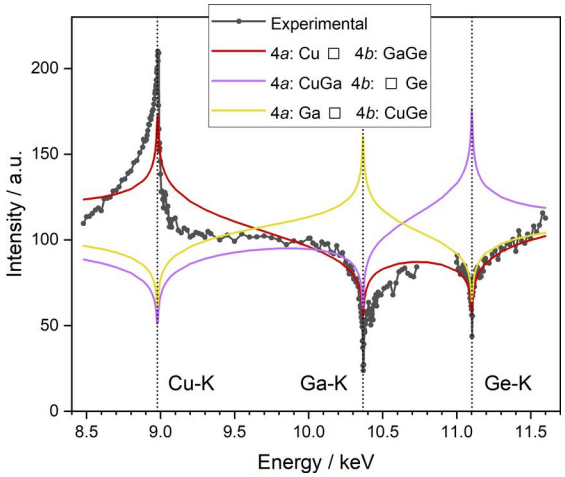

Figure 1. MEAD analysis of $CuGaGeS_4$ [3].

The energy range of 5 – 14 keV of beamline KMC-2 at BESSY II, HZB, Berlin [4] allows measurements at the absorption edges of many technically relevant elements, in particular the transition metals of the 4th period. We recently utilized this to measure $CuGaGeS_4$ (see Fig. 1) and off-stoichometric Cu_2ZnGeS_4 compounds.

Measurements on $Sn_2SbS_2I_3$ required lower energies, as the L-edges of Sn and Sb lie between 3.9 and 4.7 keV. These experiments were conducted on beamline I16 at Diamond Light Source, Didcot, UK [5], in deviation from our usual procedure using single crystals. As the measurement geometry of MEAD keeps the diffraction vector constant, the method is unaffected by preferred orientation and can be applied to samples of any degree of graininess.

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