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Element-specific atomic-scale structure and anion positions of Cu2(Zn,Fe)SnS4 kesterite-stannite alloys

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Substituting Zn by Fe in Cu₂ZnSnS₄ changes the band gap of the material from about 1.5 eV to about 1.8 eV [Shibuya et al., Appl. Phys. Lett. 104, 021912, 2014]. Interestingly, the transition from Cu₂ZnSnS₄ to Cu₂FeSnS₄ is accompanied by a change of the crystal structure from kesterite type to stannite type via a complex rearrangement of the cation species [Schorr et al., Eur. J. Mineral. 19, 65, 2007]. Furthermore, the S anions in the mixed system are surrounded by different local cation configurations. In order to determine the element-specific bond lengths of the alloy material, Cu₂(Zn,Fe)SnS₄ powder samples with 0 ≤ Fe/(Zn+Fe) ≤ 1 were investigated with extended X-ray absorption fine structure spectroscopy. All bond lengths are nearly independent of the alloy composition, yet they differ substantially for the different elements. While the Cu-S and Fe-S bond lengths are identical, the Zn-S and Sn-S bond lengths are larger by about 0.03 and 0.12 Å, respectively. Based on these experimental results, the S anion position is modelled for different cation configurations and is found to be clearly different in the Zn or the Fe containing environment. This leads to an intrinsic structural inhomogeneity of the alloys on a subnanometer scale. The impact of the S anion displacement on the band gap energy was determined by density functional theory based calculations revealing a strong correlation between local atomic arrangements and electronic properties of Cu₂(Zn,Fe)SnS₄.

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