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The kesterite –stannite structural phase transition: comparison of the series Cu2(Zn,Fe)S4, Cu2(Zn,Cd)S4 and Cu2(Zn,Mn)SnSe4

Cation/anion alloying is a well established method for band gap tailoring in compound semiconductors. In kesterite-type Cu-based quaternary chalcogenides alloying of Cu or Zn with another mono- or divalent cation is discussed to reduce Cu/Zn disorder (CuZn and ZnCu anti-sites in Cu-Zn planes at z=¼ and ¾ [2]).
Quaternary chalcogenides crystallizing in the stannite structure do not exhibit this kind of disorder. This is due to a different cation arrangement in these crystal structures.
In the presentation we discuss the solid solution series Cu2(Zn,Fe)S4 (CZFeTS,powder), Cu2(Zn,Cd)S4 (CZCdTS, monograins and thin films) and Cu2(Zn,Mn)SnSe4 (CZMnTSe, powder). The end members CZTS [2] and CZTSe crystallize in the kesterite structure, whereas CFeTS [2], CCdTS [3] and CMnTSe [3] crystallize in the stannite structure respectively. Within these series a structural transition from the kesterite to the stannite structure occurs. We performed detailed structural investigations based on neutron powder diffraction experiments which provide the cation distribution in the crystal structure allowing a distinction between iso-electronic cations Cu+ and Zn2+ as well as electronic similar cations Mn2+ and Fe2+.
A remarkable structural feature is the abrupt change of the tetragonal deformation c/2a (a and c are the lattice parameter). In the series CZFeTS and CZCdTS this change occurs at the same x value (for CZCdTS as well in monograin as in thin films). In the end member CZTS is c/2a~1, where as in the end member CZTSe is c/2a<1. Thus in the latter the c/2a value increases by substituting Zn by Mn until a value of c/2a~1 is reached.
In the CZFeTS series the kesterite-stannite transition is characterized by a cation re-distribution process [2]. We will discuss this process and the possibility of applying it to the other both series.

[1] Gurieva et al., Phys. Rev. Mat. under review

[2] Schorr et al., Europ. J. Mineral. 19 (2007) 65

[3] Schäfer et al., Z. Krist. 145 (1977) 356

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