$Cu_3Se_yTe_{1-y}$: A new representative of transition metal dichalcogenides

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Due to the enormous energy requirements of a further growing and technologized population, the research in material sciences is more and more focused on developments in "green" energy applications. Besides directly decreasing the demands of energy for any application, enhanced efficiencies can provide a further approach to minimize costs and temporary lacks. Therefore, thermoelectrics offer promising opportunities to directly convert waste heat into electrical energy. Mixed ionic or electronic conductive coinage-metal chalcogenides and chalcogenide-halides are known as promising candidates for reaching high figures of merit ZT (that describe the general thermopower of a material), which result from low thermal conductivity combined with high electronical conductivity and thereby high Seebeck coefficients [1,2].

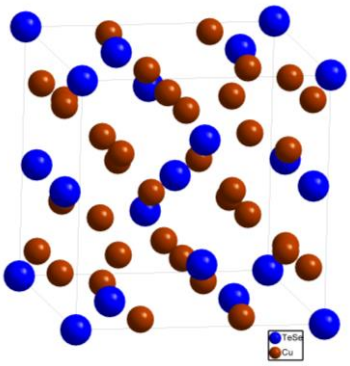

Fig. 1 Predicted structure of $Cu_3Se_{0.3}Te_{0.7}$.

With $Cu_3Se_yTe_{1-y}$ (y = 0.1 – 0.6) a new solid solution with promising structural and physical properties was established. Single and polycrystalline samples could be grown by a copper chloride supported solid-state reaction in sealed silica ampoules. Powder- as well as single crystal X-ray diffraction measurements showed that the compound crystallized in the cubic space group Pm-3n (Nr. 223) with lattice parameters a = b = c = 7.324(9) – 7.210(6) Å for y = 0.1 - 0.6. The lattice parameters as a function of the selenium content show good agreement with Vegard's law (Fig. 2). The predicted structure (Fig. 1) shows partially occupied copper positions, which could provide potential ion mobilities within the structure. Therefore, further characterization of the electronical and thermoelectric properties is required. The Seebeck values as well as the electronical conductivity are being determined. Potentiostatic electrochemical impedance spectroscopy can show phase related electrical and ion conductivity and with laser flash analysis the total thermal conductivity could be determined to calculate the overall thermoelectric power ZT.

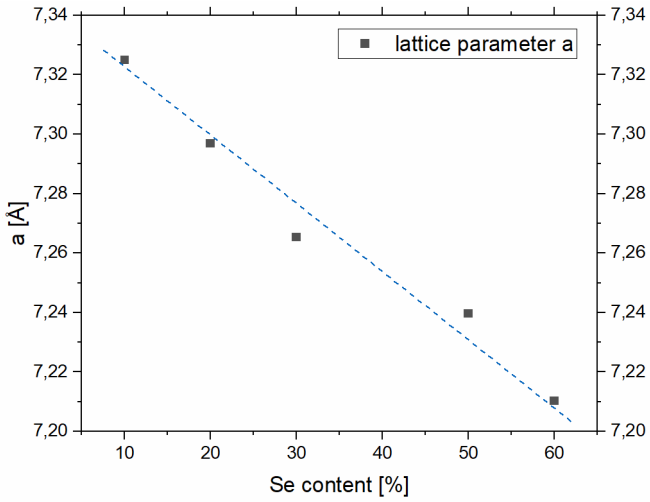

Fig. 2 Lattice parameter a in the range of y = 0.1 - 0.6 in good agreement with Vegard behaviour.

[1] A. Vogel, T. Nilges. Ion Dynamics and Polymorphism in $Cu_{20}Te_{11}Cl_3$. Inorg. Chem, 20, 15233–15241 (2021)

[2] T. Nilges *et al.* Reversible switching between p- and n-type conduction in the semiconductor $Ag_{10}Te_4Br_3$. Nature Materials, 8(2), 101-108 (2009)