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Chalcogenides for wearable thermoelectrics

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Wearable renewable energy generators are an attractive alternative to battery-based systems and can generate power up to a few Watts for portable electronic equipment. Although the most inorganic semiconductor materials are brittle at room temperature (RT) the Ag2SeTeS)1 chalcogenides show exceptional plastic deformability and high thermoelectric performance making them suitable materials for wearable thermoelectrics. In this study, we investigate ternary and quaternary Ag2(SeTeS)1 solid solutions with Se/Te doping closer to Ag2S end.

A series of samples was prepared by rapid casting: Ag2S1-xSex, Ag2S1-xTex and Ag2S0.5Te0.5-xSex (x = 0.1, 0.2, 0.3, 0.4) in to form of Ø = 3 mm, 12 mm long homogeneous ingots. Significantly high ZT = 0.47 at RT was observed for Ag2S0.7Se0.3 (so far measured by Harman method).

Ag2(S/Se)1 and Ag2(Se/Te)1 ternary systems crystalize in an orthorhombic or monoclinic structure, depending on the detailed S/Se, Se/Te atomic ratio. Addition of Te into these systems is introducing favorable cubic phase, as well observed in Ag2(S/Te)1 ternary middle region. Well known monoclinic –cubic phase transformation of Ag2(S/Se)1 [1] is pulled down to lower temperatures (even under RT) where it stabilizes with rising Te concentration. Highly disordered Ag atoms stay present in the cubic phase mimicking amorphous structure examined by diffraction.

In this contribution we present a systematic study of Ag2(SeTeS)1 chalcogenides. Temperature induced structural phase transformations are examined by differential scanning calorimetry and synchrotron in situ diffraction. Inelastic neutron scattering investigations shed light on the compounds'phonon properties showing a phonon renormalization and broadening with addition of Se/Te to Ag2S and temperature treatment. The results are backed up by density functional theory and molecular dynamics calculations. We present data from thermoelectric characterizations carried out from RT up to 200℃.

[1] Bontschewa-Mladenowa, Z. and Zaneva, K. (1977), Untersuchung des Systems Ag2Se-Ag2S. Z. anorg. allg. Chem., 437: 253-262. https://doi.org/10.1002/zaac.19774370137

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