Linking crystal structure to thermal transport in filled β-Mn-type chalcogenides

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Controlling the elastic properties of the material could become a powerful tool for tuning thermal transport in solids. Nevertheless, the impact of the crystal structure, chemical bonding, and elastic properties on the lattice thermal conductivity remains to be elucidated. This is a pivotal issue for the advancement of thermoelectric materials. In this context, the influence of cation substitution in tetrahedral voids on the structural, thermal, and thermoelectric properties of α- and β-$Pb_yGa_{6-x}In_xTe_{10}$ – filled β-manganese-type phases – is reported here [1,2]. The investigated materials show semiconducting behavior and change from *p*- to *n*-type conductivity, depending on chemical composition and temperature. Our findings indicate that the electronic transport in β-Mn-type phases is largely influenced by the substantial distortion of the Te framework which causes the low weighted mobility and strong scattering of charge carriers. The presence of a significant anharmonicity of lattice vibrations results in ultralow lattice thermal conductivity of $Pb_yGa_{6-x}In_xTe_{10}$ materials. With increasing x, κ_L decreases from 0.59 to an extremely low value of 0.36 W m^{-1} K^{-1} at 298 K due to the decreasing of bonding energy, intensifying of anharmonic thermal vibrations of atoms, and the formation of point defects [1-3]. This work demonstrates the efficacy of utilizing the crystal structure and elastic properties to regulate phonon transport in functional materials.

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The research has been supported by a grant (BPN/NSF/2023/1/00010) from Polish National Agency for Academic Exchange (NAWA) under the International Multilateral Partnerships for Resilient Education and Science System in Ukraine IMPRESS-U initiative.