Abstract Submitted
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Strong off-stoichiometry and large Grüneisen parameter in $AgSbTe_2$: a first principles study[1] SERGEY V. BARABASH, VIDVUDS OZOLINS, University of California, Los Angeles, MICHELE D. NIELSEN, JOSEPH P. HEREMANS, The Ohio State University — We use first-principles density-functional theory calculations to study the dynamical and compositional instabilities in $AgSbTe_2$, and compare the theoretical predictions to the results of an experimental investigation. For pure $AgSbTe_2$, some native defects, particularly Ag vacancies, have negative formation energies for a wide range of experimental conditions, thus forming in high concentrations even at low T. This leads to large deviations from the formal stoichiometry, in agreement with experimental results. Substantial deviations of the $AgSbTe_2$ phase field away from the isoplethal Ag_2Te-Sb_2Te_3 section may be expected, potentially explaining the contradictions in the low-temperature regions of the previously published phase diagrams. We estimate the defect concentrations and the resulting intrinsic doping levels under various experimental conditions. Finally, we demonstrate that the stoichiometric $AgSbTe_2$ is at the verge of a dynamical instability: the energies of acoustic phonons near the L point depend strongly on volume, changing sign at nearly the experimental volume. This leads to an unusually large value of the Grüneisen parameter, in agreement with experiment.

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Sergey Barabash
Univ. of California, Los Angeles

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