

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-

Principles Theory of Ordering, Phase Separation, and Phonon Scattering in Thermoelectric LAST (Lead-Antimony-Silver-Telluride) alloys¹

SERGEY V. BARABASH, VIDVUDS OZOLINS, UCLA, CHRIS WOLVERTON, Northwestern University — Bulk LAST ($\text{Pb}_{2-x-y}\text{Ag}_y\text{Sb}_x\text{Te}_2$) alloys exhibit* high thermoelectric figure of merit ($ZT \sim 2$ at 800K, considerably exceeding ZT of pure PbTe or AgSbTe₂), and nano-scale inhomogeneities, origin of which is poorly understood. The atomic structure of the nano-regions, as well as that of the pure AgSbTe₂, remains the subject of an experimental debate. Using density-functional theory (DFT), we calculate the composition-temperature phase diagram and vibrational spectra of $\text{Pb}_{2-x-y}\text{Ag}_y\text{Sb}_x\text{Te}_2$ alloys. We predict that the experimentally observed nanoscale inhomogeneities are due to the precipitation of ordered AgSbTe₂ phases. Two types of cation order type closely compete in AgSbTe₂, the dominant order type being D4; the predicted hypothetical order-disorder transition temperature exceeds the melting temperature of pure AgSbTe₂. The miscibility gap between solid PbTe and AgSbTe₂ phases is highly asymmetric, with a high solubility of PbTe in ordered AgSbTe₂. We also characterize the shape of coherent precipitates. Finally, the phonon spectra of AgSbTe₂ and PbTe suggest that boundary scattering of acoustic phonons causes the observed suppression of thermal conductivity. *K.F. Hsu *et al.*, Science **303**, 818 (2004).

¹supported by NSF Grant No.DMR-0427638 and by MARCO FC FENA

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Date submitted: 04 Feb 2008

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