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) alloys[1]

SERGEY V. BARABASH, VIDVUDS OZOLINS, UCLA, CHRIS WOLVERTON, Northwestern University — Bulk LAST ($Pb_{2-x-y}Ag_ySb_xTe_2$) alloys exhibit* high thermoelectric figure of merit (ZT$\sim$2 at 800K, considerably exceeding ZT of pure PbTe or $AgSbTe_2$), and nano-scale inhomogeneities, origin of which is poorly understood. The atomic structure of the nano-regions, as well as that of the pure $AgSbTe_2$, remains the subject of an experimental debate. Using density-functional theory (DFT), we calculate the composition-temperature phase diagram and vibrational spectra of $Pb_{2-x-y}Ag_ySb_xTe_2$ alloys. We predict that the experimentally observed nanoscale inhomogeneities are due to the precipitation of ordered $AgSbTe_2$ phases. Two types of cation order type closely compete in $AgSbTe_2$, the dominant order type being D4; the predicted hypothetical order-disorder transition temperature exceeds the melting temperature of pure $AgSbTe_2$. The miscibility gap between solid PbTe and $AgSbTe_2$ phases is highly asymmetric, with a high solubility of PbTe in ordered $AgSbTe_2$. We also characterize the shape of coherent precipitates. Finally, the phonon spectra of $AgSbTe_2$ 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).

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

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Date submitted: 04 Feb 2008 Electronic form version 1.4