Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Nanoscale clusters in the thermoelectric $AgPb_mSbTe_{m+2}$ and $Ag_nSn_mSb_nTe_{m+2n}$ materials[1] HE LIN, EMIL BOZIN, KHANG HOANG, S.D. MAHANTI, SIMON BILLINGE, Department of Physics and Astronomy, Michigan State University, ERIC QUAREZ, JOHN ANDROULA, MERCOURI KANATZIDIS, Department of Chemistry, Michigan State University — The local structure of the $AgPb_mSbTe_{m+2}$ series of high performance thermoelectric materials has been studied using the atomic pair distribution function (PDF) method. The dimensionless thermoelectric figure of merit, ZT, of the $m \sim 18$ composition material was found to reach 1.7 at 700 kelvin, compared to the highest observed ZT of only 0.84 for PbTe at 648 kelvin in n-doped material. This is asurprisingly large enhancement in ZT for the addition of just 10%per formula-unit of silver and antimony ions. It is clearly of the greatest importance to trace the origin of the ZT enhancement. Three candidate-models were attempted for thestructure of this class of materials using either a one-phase or a two-phase modeling procedure. Combining modeling the PDF with HRTEM data we show that $AgPb_mSbTe_{m+2}$ contains nanoscale inclusions with composition close to $AgPb_3SbTe_5$ randomly embedded in a PbTe matrix. We extended the local structural PDF study to $Ag_nSn_mSb_nTe_{m+2n}$, preliminary results of which suggest the presence of nanoscale inclusions in this system as well.

[1]NSF NIRT grant DMR-0304391

He Lin
Department of Physics and Astronomy,
Michigan State University, East Lansing, MI 48824

Date submitted: 29 Nov 2005 Electronic form version 1.4