Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Microstructure and Nucleation Mechanism for Nanoprecipitates in PbTe-AgSbTe$_2$[1] XUEZHI KE, University of Nevada, Las Vegas; East China Normal University, CHANGFENG CHEN, University of Nevada, Las Vegas, JIHUI YANG, General Motors, LIJUN WU, JUAN ZHOU, QIAN LI, YIMEI ZHU, Brookhaven National Laboratory, PAUL R.C. KENT, Oak Ridge National Laboratory — Many recent advances in thermoelectric (TE) materials are attributed to their nanoscale constituents. Determination of the nanocomposite structures has represented a major experimental and computational challenge and eluded previous attempts. Here we present the first atomically resolved structures of high performance TE material PbTe-AgSbTe$_2$ by transmission electron microscopy imaging and density functional theory calculations. The results establish an accurate structural characterization for PbTe-AgSbTe$_2$ and identify the interplay of electric dipolar interactions and strain fields as the driving mechanism for nanoprecipitate nucleation and aggregation, which provides key insights for understanding a broad class of complex nanocomposite materials.

[1]This work was supported by DOE under DE-FC52-06NA26274 (UNLV), DE-FC26-04NT42278 (GM) and DE-AC02-98CH10886 (BNL). It also used resources at the National Center for Computational Sciences and the Center for Nanophase Materials Sciences at ORNL.

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Date submitted: 18 Nov 2008 Electronic form version 1.4