Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic Inhomogeneity in PbTe-based High Performance Thermoelectric Materials Observed by NMR E.M. LEVIN, K. SCHMIDT-ROHR, B.A. COOK, Ames Laboratory DOE and Iowa State University, M.G. KANATZIDIS, Northwestern University — Effects of composition and synthesis conditions on the local structure and charge carrier concentration in $Ag_xSb_yPb_{18}Te_{20}$ (LAST-18) thermoelectric (TE) materials have been studied by ^{125}Te and ^{207}Pb nuclear magnetic resonance (NMR) with magic-angle spinning. The high-resolution ^{125}Te NMR spectra show that most Sb and Ag is not part of Sb_2Te_3, $AgSbTe_2$, or Ag_2Te inclusions. Biexponential NMR spin-lattice (T_1) relaxation as well as Knight shifts of ^{125}Te and ^{207}Pb NMR signals show that many LAST-18 materials contain two phases of similar composition but with free electron concentrations that differ by more than an order of magnitude, i.e. these materials are electronically inhomogeneous. The NMR data were calibrated against Hall- and Seebeck-effect measurements to give the charge carrier concentrations in the two phases. This electronic inhomogeneity may result in the appearance of potential barriers inside TE materials, similar to those observed for semiconductor-semiconductor or metal-semiconductor junctions. Such barriers may affect thermopower, electrical, and thermal conductivity of TE materials.

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Date submitted: 29 Nov 2008 Electronic form version 1.4