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New Insights into High-Performance Thermoelectric Tellurides from ^{125}Te NMR Spectroscopy E.M. LEVIN, Y.-Y. HU, B.A. COOK, J.L. HARRINGA, K. SCHMIDT-ROHR, Ames Laboratory DOE and Iowa State University, M.G. KANATZIDIS, Northwestern University — Thermoelectric materials are widely used for direct transformation of heat to electricity (Seebeck effect) and for solid state refrigeration (Peltier effect). Efforts to increase the efficiency of high-performance thermoelectrics, which include narrow-gap, doped tellurium-based semiconductors, require detailed knowledge of their local structure and bonding. We have used ^{125}Te nuclear magnetic resonance (NMR) as a local probe for obtaining better understanding of these high-performance thermoelectric tellurides, specifically PbTe doped with Ag and Sb (LAST materials) and GeTe doped with Ag and Sb (TAGS materials). The resonance frequencies and line shapes of the NMR spectra, as well as spin-lattice relaxation times and chemical shift anisotropies are highly sensitive to the composition and synthesis conditions of LAST and TAGS materials, enabling studies of the *local* composition, distortion, bonding, and carrier concentration. Several intriguing phenomena including electronic inhomogeneity and local distortions of the crystal lattice have been observed by NMR.

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