

Abstract Submitted  
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**High-Resolution  $^{125}\text{Te}$  NMR of Novel Thermoelectric Materials**

E.M. LEVIN, K. SCHMIDT-ROHR, B.A. COOK, Ames Laboratory DOE and Iowa State University, MI-KYUNG HAN, M.G. KANATZIDIS, Northwestern University — Several novel Te-based thermoelectric materials with extraordinary figure of merit  $ZT \geq 1.4$  have been studied by high-resolution 25 kHz magic angle spinning  $^{125}\text{Te}$  nuclear magnetic resonance (NMR) in order to investigate variations in composition on the nano-scale. A 20-fold wider  $^{125}\text{Te}$  NMR signal of both  $\text{AgSbGe}_4\text{Te}_6$  and  $\text{AgSbGe}_{5.67}\text{Te}_{7.67}$  ( $\sim 90$  kHz) compared to that of  $\text{PbTe}$  (4.5 kHz) indicates a variation of shifts due to local composition fluctuations. The similar total shift of the main peak in  $\text{Ag}_{0.53}\text{Pb}_{18}\text{Sb}_{1.2}\text{Te}_{20}$  (-1790 ppm) and  $\text{PbTe}$  (-1750 ppm) and similarly long  $T_2$  relaxation time show that the majority of Te atoms in both materials has a similar environment. A second peak in  $\text{Ag}_{0.53}\text{Pb}_{18}\text{Sb}_{1.2}\text{Te}_{20}$  at -1600 ppm shows the presence of a second type of Te site, accounting for  $\sim 1/3$  of all Te. These are apparently located in {Ag,Sb}-rich inclusions, as indicated by a much shorter  $T_2$ , which can be due to the effect of quadrupolar relaxation of  $^{121}\text{Sb}$  or  $^{123}\text{Sb}$  (spin 5/2 or 7/2, respectively) on  $^{125}\text{Te}$ . Our data confirm suggestions made by Hsu *et al.*, Science (2004) and by Chen *et al.*, Appl. Phys. Lett. (2005) about the presence of nano-scale inclusions in  $\text{Ag}_{0.53}\text{Pb}_{18}\text{Sb}_{1.2}\text{Te}_{20}$ , which result in low lattice thermal conductivity and high  $ZT$ .

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