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Reassessment of the carrier concentration in GeTe-based thermoelectric materials by ^{125}Te NMR E.M. LEVIN, J.D. ACTON, K. SCHMIDT-ROHR, Ames Laboratory US DOE and Iowa State University — $Ge_{1-x}Ag_{x/2}Sb_{x/2}Te$ p-type thermoelectric materials ("TAGS-n") were studied extensively in the 1970s and then again recently. They exhibit an unusual combination of large thermopower, S, and high hole concentration, p, reported based on the Hall effect data, which has not been explained. To solve this puzzle, we have synthesized GeTe, GeTe:Bi, and TAGS-n with n= 97, 94, 90, and 85 and studied XRD, thermopower, electrical resistivity, thermal conductivity, and ^{125}Te NMR. Most importantly, we have determined the carrier concentrations using ^{125}Te NMR spin-lattice relaxation and Knight shift. In GeTe and GeTe:Bi, we found that carrier concentrations generally agree with the values reported from Hall effect. In TAGS-n, they are much lower but agree better with the values expected from S vs. p for GeTe-based materials, solving the puzzle partially. The NMR vs. Hall effect discrepancy in TAGS-n can be due to the presence not only of holes but also electrons generated by Sb atoms, which results in artificially high hole concentration from Hall effect. Even though the true hole concentration is lower than reported, the thermopower of TAGS-n is still significantly larger than that of GeTe and GeTe:Bi at similar carrier concentration. This can be explained by energy filtering enhanced by potential barriers formed due to Ag-Sb pairs in the TAGS-n lattice.

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