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**Effects of Ge replacement in GeTe by Ag or Sb on the Seebeck coefficient and carrier concentration modified by local electron imbalance**

E.M. LEVIN, A. HOWARD, U.S. DOE Ames Laboratory and Iowa State University, W.E. STRASZHEIM, Iowa State University — XRD, SEM, EDS,  $^{125}\text{Te}$  NMR, Seebeck coefficient, and electrical resistivity of  $\text{Ag}_x\text{Ge}_{50-x}\text{Te}_{50}$  and  $\text{Sb}_x\text{Ge}_{50-x}\text{Te}_{50}$  alloys have been studied. Replacement of Ge in GeTe by Sb significantly increases the Seebeck coefficient, while replacement by Ag decreases it. These effects can be attributed to a change in carrier concentration observed via  $^{125}\text{Te}$  NMR spin-lattice relaxation measurements and NMR signal position, which mostly depends on the Knight shift. Variation in carrier concentration in  $\text{Ag}_x\text{Ge}_{50-x}\text{Te}_{50}$  and  $\text{Sb}_x\text{Ge}_{50-x}\text{Te}_{50}$  can be attributed to different electron configurations of valence electrons of Ag ( $4d^{10}5s^1$ ) and Sb ( $5s^25p^3$ ) compared to that of Ge ( $4s^24p^2$ ) resulting in local electron imbalances and changing the concentration of charge carrier (holes) generated by Ge vacancies. In contrast, our  $^{125}\text{Te}$  NMR and Seebeck coefficient data for  $\text{Ag}_2\text{Sb}_2\text{Ge}_{46}\text{Te}_{50}$  are similar to those observed for GeTe. This shows that effects from Ag and Sb compensate each other and indicates the existence of [Ag+Sb] pairs. The effects of Ge replacement in GeTe by Ag, Sb, or [Ag+Sb] on rhombohedral lattice distortion also have been analyzed. Interplay between the Seebeck coefficient and electrical resistivity in these alloys results in variation of power factor; the value of 45 mW/cm K<sup>2</sup>, the highest among known tellurides, was found for  $\text{Sb}_2\text{Ge}_{48}\text{Te}_{50}$ .

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