Enhanced Thermoelectric Properties of Ge-doped n-type Bi_2O_2Se Ceramics

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Increasing global energy consumption and the negative environmental impacts of many current energy conversion technologies, such as the combustion of fossil fuels, has led to increased activity in developing alternative energy conversion technologies. Thermoelectric (TE) conversion of waste heat into electricity is one of them. The dimensionless figure of merit ZT is a measure of the applicability of a material [1]. $ZT = S^2\sigma T/\kappa$, where S is thermopower (Seebeck coefficient), σ is electrical conductivity, κ is thermal conductivity, and T is thermodynamic temperature. Accordingly, thermoelectric materials show high electrical conductivity, low thermal conductivity and high levels of thermopower simultaneously. Such materials are, however, rarely found because these three parameters cannot be controlled independently, as they are functions of the Fermi level (and other parameters) in conventional semiconductors.

Ceramic samples with the composition $Bi_{2-x}Ge_xO_2Se_{1,01}$ (x = 0, 0.05, 0.075 and 0.1) were synthesized by solid-state reaction and compacted using a hot-pressing technique. The prepared materials were characterized by XRD analysis, electron microscopy and measurements of electrical conductivity σ, Seebeck coefficient S, and thermal conductivity κ in the temperature range 300-780 K. Ge in the Bi_2O_2Se host structure led to an increase of the free electron concentration compared to pristine $Bi_2O_2Se_{1.01}$. The increase is explained in terms of the formation of point substitutional defects (donors) in the Bi sublattice - Ge_{Bi}^{+}, producing free electrons. As a result, we observe an increase in the lectrical conductivity and decrease in Seebeck coefficient while thermal conductivity changes slightly. The highest value of the dimensionless figure of merit $ZT = \sigma S^2T/\kappa$ reaches 0.25 for the composition $Bi_{1,95}Ge_{0,05}O_2Se_{1,01}$ at T=724 K, which is, to date, the highest ZT value reported for Bi_2O_2Se ceramics. Our results suggest that Bi_2O_2Se is still worth exploring.

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[1] G.S. Nolas, J. Sharp, H.J. Goldsmid, Thermoelectrics, Basic principles and New Materials Developments (Berlin Heidelberg, Springer, 2001).