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Enhancement of the Thermoelectric Performance of $Bi_{0.4}Sb_{1.6}Te_3$ Alloys by In and Ga Doping

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We report an enhancement of the thermoelectric figure of merit in polycrystalline In- and Ga-doped $Bi_{0.4}Sb_{1.6}Te_3$ compounds. Via the controlled doping of In or Ga, the lattice thermal conductivity was effectively reduced by strong point-defect phonon scattering while the power factor was not significantly changed due to the similarity of the density of states near the valence-band maximum between undoped and In- or Ga-doped compositions. An enhanced ZT of 1.2 at 320 K was obtained in 0.5 at.% In-doped $Bi_{0.4}Sb_{1.6}Te_3$ compound by these synergetic effects.

Key words: Thermoelectric, $Bi_{0.4}Sb_{1.6}Te_3$, lattice thermal conductivity, point defect, power factor

INTRODUCTION

Recently, the thermoelectric performance of Bi-Te-based thermoelectric materials has been remarkably enhanced through the newly developed processing technology of nanostructuring.[1–10] Advances in theories and experiments related to nanostructured thermoelectric materials confirm that the enhanced ZT ($=\sigma S^2 T/\kappa$) in nanostructured thermoelectric materials is mainly due to the reduced lattice thermal conductivity κ_{lat} ($=\kappa_{tot} - \kappa_{ele}$) caused by interface phonon scattering, where σ is the electrical conductivity, S is the Seebeck coefficient, κ_{tot} is the total thermal conductivity, and κ_{ele} is the electronic contribution to κ_{tot} at a given absolute temperature (T); For example, Poudel et al.[11] reported a peak ZT of 1.4 at 100°C by fabricating nanograined composite p-type $Bi_{2-x}Sb_xTe_3$ via high-energy ball milling and hot pressing.

On the other hand, the substitutional doping approach has been shown to be one of the most effective ways to improve the thermoelectric figure of merit because this approach can either reduce the κ_{lat} value by strong point-defect phonon scattering or enhance the power factor (σS^2) through a modification of the electronic structures via density of states (DOS) engineering. It was experimentally found that a few dopants, such as Al, Ga, In, Cu, and Ag, effectively increase the ZT of p-type Bi-Sb-Te compounds mainly due to the reduced κ_{lat}.[12–16] The reduction of κ_{lat} in doped Bi-Sb-Te compositions likely originates from the strong point-defect phonon scattering in the presence of substitutional doping elements. However, there exists much uncertainty about which dopants can enhance the carrier transport properties pertaining to σ and S. Recently, Lv et al. proposed that enhanced thermoelectric performance can be obtained in doped $Bi_{0.5}Sb_{1.5}Te_3$ compounds by chemical potential tuning.[17] They presented first-principles calculations related to the enhancement of the power factor and suggested many promising candidate materials with high ZT values (a peak ZT = 1.8 at 300 K) including In- and Ga-doped $Bi_{0.5}Sb_{1.5}Te_3$.

In this study, we present experimental evidence of the In- and Ga-doping effect in bulk polycrystalline $Bi_{0.4}Sb_{1.6}Te_3$. We also perform first-principles calculations for In- and Ga-doped $Bi_{0.5}Sb_{1.5}Te_3$ compounds in order to understand the effect of doping elements on the DOS near the valence-band maximum. A reduced value of κ_{lat} and an optimized

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