Effect of Se Substitution on Structural and Electrical Transport Properties of $Bi_{0.4}Sb_{1.6}Se_{3x}Te_{3(1-x)}$ Hexagonal Rods

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In the current study, novel hexagonal rods based on $Bi_{0.4}Sb_{1.6}Te_3$ ingots dispersed with x amount of Se (x = 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0) in the form $Bi_{0.4}Sb_{1.6}Se_{3x}Te_{3(1-x)}$ were synthesized via a standard solid-state microwave route. The morphologies of these rods were explored using field-emission scanning electron microscopy (FESEM). The crystal structure of the powders was examined by x-ray diffraction (XRD) analysis, which showed that powders of the $0.0 \leq x \leq 0.8$ samples could be indexed to the rhombohedral phase, whereas the sample with x = 1.0 had an orthorhombic phase structure. The influence of variations in the Se content on the thermoelectric properties was studied in the temperature range from 300 K to 523 K. Alloying of Se into $Bi_{0.4}Sb_{1.6}Te_3$ effectively caused a decrease in the hole concentration and, thus, a decrease in the electrical conductivity and an increase in the Seebeck coefficient. The maximal power factor measured in the present work was 7.47 mW/mK^2 at 373 K for the x = 0.8 sample.

Key words: Quaternary alloy systems, thermoelectric properties, solid-state microwave synthesis, x-ray diffraction

INTRODUCTION

Narrow-gap binary chalcogenides, such as Bi_2Te_3, Sb_2Te_3, and Bi_2Se_3, are well known as thermoelectric (TE) materials for use in thermoelectric generators operating at room temperature (300 K).[1–3] The crystal structures of these chalcogenides are rhombohedral, with space group $D_{3d}^5(R\bar{3}m)$. These crystal structures can be represented as a stack of hexagonally arranged atomic planes, each consisting of only one type of atom. Five atomic planes are stacked in a close-packed manner, with a $Te^I(Se^I)$–$Bi(Sb)$–$Te^{II}(Se^{II})$–$Bi(Sb)$–$Te^I(Se^I)$ arrangement.[4,5] These complex crystal structures and the disordered atomic distributions, which yield exceptionally low lattice thermal conductivity, contribute significantly to the excellent TE properties of these materials.[6]

TE materials convert thermal energy directly into electrical energy or vice versa, as in power generation or refrigeration. The efficiency of a TE material is conventionally defined by its dimensionless figure of merit (ZT), where $ZT = \sigma S^2 T/k$, and T, S, σ, and k are the absolute temperature, Seebeck coefficient, electrical conductivity, and thermal conductivity, respectively. An ideal TE material should have the combination of high power factor (σS^2) and low thermal conductivity. ZT is very sensitive to variations in composition, suggesting that ZT could be improved by decreasing the lattice thermal conductivity through enhanced phonon scattering attributable to lattice distortion.[7–9]

In recent years, ternary and quaternary chalcogenides containing heavy atoms have been developed as materials with high-performance bulk TE properties, having isotropic complex structures that are beneficial for the large carrier effective masses and low lattice thermal conductivity associated with such systems.[10] Most compounds are stable in an environment when they can combine with a set of properties that make them appropriate for practical TE applications. Given the versatility in the choice of suitable electronegativity of the chalcogen elements,