Studies on electrical and thermal transport properties in In_4Se_3 based materials and composites for thermoelectric applications

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Abstract

Direct conversion of heat to electrical energy using the Seebeck effect has a lot of potential in power generation. The widespread use of thermoelectric devices in everyday life is currently impractical due to their low conversion efficiency. So, the present work is carried out with an aim to improve the thermoelectric figure of merit (ZT) of n-type indium selenide (n-In_4Se_3) by tuning the carrier transport through the introduction of doping and microstructure modifications. To achieve a high ZT, thermal conductivity needs to be reduced with simultaneous enhancement of the power factor ($S^2\sigma$, where S is the Seebeck coefficient and σ is electrical conductivity) or at least the latter should remain unchanged. Thus, in this work, the following three strategies were adopted, viz. (i) inclusion of indium nanoparticles together with Se-deficiency in In_4Se_3, (ii) iodine doping, and (iii) introduction of SnSe nanostructure in In_4Se_3. Moreover, density functional theory based calculations were performed to understand the structure property relationship in In_4Se_3. It is found that Se-deficiency and presence of indium nanoparticles in In_4Se_{3-x} reduced the thermal conductivity due to enhanced phonon scattering by point defects and nanoparticles in the system. At the same time, the power factor is also found to increase due to increased carrier concentration. For further improvement of carrier concentration, In_4Se_3 was doped with iodine. This has increased the electrical conductivity which leads to enhanced power factor in $In_4Se_{3-x}I_x$ compared to In_4Se_3. Simultaneously, the thermal conductivity is also found to reduce appreciably due to the effects of atomic mass fluctuations and grain boundaries. On the other hand, in a sample having phase separated composite of In_4Se_3 with SnSe, the thermal conductivity is found to be reduced significantly with a value of 0.54 W/m-K at 300 K due to scattering of low-and mid-frequency phonon and low energy charge carrier filtering at the heterojunction between In_4Se_3/SnSe. The electrical and thermoelectric transport parameters in n-In_4Se_3 were measured in the present study in the temperature range 300 – 700 K. The lowest value of the thermal conductivity was observed in In_4Se_3 samples with SnSe heterojunctions whereas the highest value of ZT was found in Se-deficient In_4Se_3 with indium nanoinclusions, both at 700 K. Attempt has also been made in this study to analyze the structure-property correlation theoretically using local spin density and generalized gradient approximation in iodine doped samples on the basis of density functional theory.

Keywords: Seebeck coefficient, thermoelectric, thermal conductivity, indium selenide, nanoinclusion