Thermal stability and thermoelectric performance of single-crystalline *β*-Zn_xSb_3

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Abstract

The β-Zn_4Sb_3 possess low thermal conductivity and high thermoelectric (TE) performance, which is considered as a cost-effective *p*-type TE material in the temperature range of 500-750 K Nevertheless., its poor thermal stability at above 623 K has been the roadblock to commercial application. The solution depends on the realization of intrinsic properties of β-Zn4Sb3, such as chemical stoichiometry and crystal structure that can develop appropriate strategy to improve the TE performance and thermal stability. Herein we synthesize single-crystalline Zn_xSb_3 (x = 3.67, 3.82, 3.97 and 4.14) by Bridgman method and observe the temperature-dependent TE property, crystal structure and phase transition with varying x. Among these single crystals, the $Zn_{4.14}Sb_3$ reveals a single-phase of β-Zn_4Sb_3 with astonishing thermal stability at high temperature. On the contrary, the $Zn_{3.67}Sb_3$ shows the secondary ZnSb precipitate, which makes it unstable. Most importantly, the $Zn_{4.14}Sb_3$ sample has lower thermal conductivity (~ 0.9 W m^{-1} K^{-1}) and lower electrical resistivity ρ ~ 2 (m Ω*cm) and its figure of merit ZT reaches ~0.75 at 623 K.