Development of High Performance Nanocrystalline Bi0.8CuxSb(1.2-x)Te3 Thermoelectric Films Using Advanced Pulsed Laser Deposition

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Bi2Te3-based materials have exhibited high thermoelectric performance, particularly at lower temperatures making them suitable for cooling applications. However, their efficiency is limited by the early onset of intrinsic excitation of minority charge carriers. This work reports a high thermoelectric performance of copper-doped nano-crystalline p-type Bi0.8Sb1.2Te3 films prepared by pulsed laser deposition. Typically, a ZT of 1.4 at 300 K was realized in the Bi0.8Sb1.2Te3-2Cu film sample. The high figure of merit was achieved from the simultaneous increase in the power factor and decrease in the thermal conductivity caused by intermediate copper doping. DFT calculations revealed an increase in the bandgap of the material with Cu-concentration and suggested that Cu preferentially replaces Sb in the Bi/Sb sites, an assertion which was confirmed by the energy dispersive spectroscopy (EDS) result. The Cu-doping facilitated an increase in the majority hole concentration, thus suppressing the intrinsic excitation and improving the Seebeck coefficient. Also, the dispersed Cu atoms at the interfacial grain boundaries emanating from the PLD-supported alternate deposition feature facilitated selective blockage of less-energetic charge carriers, thereby increasing the Seebeck coefficient through carrier filtering effect. The nano- dispersed Cu atoms near the grain boundaries, together with the doping-induced point defects, caused enhanced wide-spectrum phonon scattering, leading to a decline in the lattice thermal conductivity, thus improving the figure of merit. The results presented here represent a significant breakthrough in the development of thermoelectric materials.

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