Abstract

The main focus of this thesis is to improve the thermoelectric figure of merit (zT) of PbTe by tuning the carrier transport mechanism through the introduction of nanostructures and impurity bands. For higher thermoelectric figure of merit, its power factor ($= S^2\sigma$, where S and σ are the thermopower and electrical conductivity, respectively) need to be enhanced or at least remained unaffected with the reduction in thermal conductivity (κ). For the reduction of thermal conductivity, transport properties in porous nanogranular n-type bulk PbTe have been investigated. The porous nature of the nanograined microstructure is found to reduce the thermal conductivity significantly, however, the benefit is not found to be significant enough to overcome the observed loss in the electrical conductivity. For harnessing the beneficial effects of random atomic mass fluctuations on thermal conductivity, thermoelectric properties in n-type $PbSe_{0.5}Te_{0.5}$ have been investigated. The combined effects of atomic mass fluctuation and PbTe/PbSe endotaxial nanostructures (formed due to stoichiometric imbalance by PbI_2 doping) are found to reduce the value of the lattice thermal conductivity appreciably (≤ 1.6 $Wm^{-1}K^{-1}$) in the material system. As a result, thermoelectric figure of merit with a value of 1.5 is achieved at 625 K. For the experimental observation of the theoretically predicted Zn resonance states and its effect on thermoelectric properties in PbTe, transport properties in endotaxially nanostructured n-type PbTe:ZnTe have been investigated. No evidence of Zn resonance level have been observed up to a carrier concentration of 4.17×10^{19} cm^{-3}. A significant reduction in lattice thermal conductivity has been observed due to increased scattering of long wavelength phonons by ZnTe nanostructures and as a result enhancement in figure of merit, with a maximum value of 1.35 at 650 K, is observed. For high thermoelectric performance, an alternative approach for carrier concentration optimization has been demonstrated in Yb doped p-type $Pb_{1-x}Sn_xTe$. The temperature dependent redistribution of electrons between the Yb-impurity levels and the valence band is found to compensate the excess hole concentration at low temperature and negate the effect of intrinsic conduction at higher temperature leading to significantly enhanced thermopower and power factor in $Pb_{1-x}Sn_xTe$. However, the benefits of Yb-impurity levels observed in p-type $Pb_{1-x}Sn_xTe$, could not be realized in n-type $PbTe_{1-x}I_x$ due to the Fermi level pinning and increased scattering sites of the charge-carriers.

Keywords: Thermoelectric, lead telluride, nanograin, atomic mass fluctuation, endotaxial nanostructure, impurity levels.