Abstract

There has been a constant search for thermoelectric materials with higher power conversion efficiency to enhance waste heat recovery. Efficiency of a thermoelectric material is calcu- lated as figure of merit ($ZT = S^2 \sigma T / \kappa$ where $S^2 \sigma$ is power factor and κ is thermal con- ductivity). The expedition for exploring better thermoelectric performance among a copious number of materials is based either on finding a new material or on modifying the thermo- electric properties of existing ones. To enhance the thermoelectric performance of already existing materials, different methods have been used like nanostructuring, doping, rattling atoms, alloying etc. These methods either target at modifying the electronic band structure to enhance the power factor, or on the other hand, steering the phonon scatterings to reduce the thermal conductivity. In result, it increases the overall performance based on the strategy of “Phonon glass electron crystal”. Thermal conductivity is one of the dominant parame- ters for efficiency optimization. Besides the intrinsic properties, alloying and nanostructuring have been found to be very effective in controlling the thermal conductivity in large range of materials. Apart from promising low-cost binary thermoelectric materials (CdSe, PbTe etc), only a few ternary MZX (M=group IX, X; Z= Group V; X is chalcogenide) chalcogenides such as CoSbS, NiSbS, FeSbS have been studied for thermoelectric applications. Thermo- electric performance of ternary pnictide chalcogenide of d 8 transition metal materials PdPS, CoAsS have been investigated in this thesis work. A worth appraised values of ZT have been calculated for these materials. Thermoelectric figure of merit calculated for PdPS is very significant in the nano regime and due to its layered structure, it will be having many applications in the field of biology, space, computers etc. Another very important application of this research is in the thermoelectric modules in which the provision to use both legs of the module from CoAsS alloy can be possible. A significant reduction in the lattice ther- mal conductivity of type-I clathrate $Ba_8Cu_6Si_{40}$ by introducing alloy scattering and boundary scattering is observed which can be useful for many Si based technologies.