- **Thermoelectric Materials**

Efforts are going on to grow and characterize some important thermoelectric materials. The thermoelectric effects can be used for the direct conversion of thermal into electric energy. Thermoelectric devices take advantage of the fact that removing an electron from a metal requires a different amount of energy depending on the type of metal. The electrons have different energies depending on what metal they're in. If electrons with low energy flow from a metal into a metal whose electrons are of high energy, each electron has to get the energy from somewhere. The energy comes from thermal energy, and so the junction becomes cool. The reverse is also possible. Thermoelectric materials a have a wide range of uses.

The research interests on thermoelectric materials and devices based on them are growing enormously as they can be the potential alternate power sources in the near future. Also, thermoelectric devices are highly reliable, silent, light-weighted etc. The materials used for these devices should be cost effective and more importantly, efficient too.

Numerous efforts have been made to find and prepare materials with high Seebeck coefficient and hence high figure of merit given by ZT = S2Tσ/κ., where σ is the electrical conductivity, κ is the thermal conductivity, S is the Seebeck coefficient (dV/dT) and T is the temperature. Bi2Te3 and Bi2Se3 and their solid solutions are supposed to be the conventional thermoelectric materials. But several other compounds have also been tested for high performance and to improve the figure of merit, for example, CsSbBi3Te6, CsSnBi3Te6, CsPb2Bi2Te7, CsSn2Bi2Te7, Mg2Si1-xGex, Nb3SbxTe7-x, Pb1-xGexTe, PbTe, Cd1-xZnxTe, ZrNiSn, InSb etc. Materials with high Seebck coefficient, high electrical conductivity and low thermal conductivity are the candidates for producing high thermoelectric power. Electron-Phonon decoupling is the key for producing high thermoelectric figure of merit ZT, i.e., the Wiedemann-France ratio should be as high as possible. Materials with loosely bound atoms and high thermal parameters can scatter phonons much effectively than electrons. At the same time the electrons should not be disturbed as for phonons, because high electrical conductivity is also needed. Systems with high concentration charges (for high electrical conductivity), but with localized charges (for the prevention of phonon movement) are also supposed to be good thermo electric materials. Heavily doped systems will have more disorderness and hence they will reduce propagation of phonons.

In this work, some thermoelectric materials starting with Bi1-xSbx with various concentrations of x have been grown using melt growth techniques. Other systems proposed to be studied are the following ; Si1-xGex, Zn4Sb3-Cd4Sb3 system and their solid solutions, Bi2Te3 doped with Sn, Sb2Te3, Mg2Si, Mg2Sn, Mg2Pb, Mg2Ge, Mg2Sn1-x,Pbx, Mg2Ge1-xSnx, Mg2Si1-xGex, As2Te3, Ca0.8Al0.2 (metallic glass), Pb1-xGexTe, Bi2Te2.85Se0.15 doped with Cu. Preparation and characterization of all of these materials is not the scope of the present research work, only 3 to 4 series of systems will be grown and characterized.

The physical characterization techniques will involve Measurement of (1) Seebeck coefficient (the Seebeck coefficient is expected to be negative for a n-type thermoelectric material (electron doped) and positive for a p-type material (hole doped)) (2) Electrical conductivity Vs temperature (3) Thermal conductivity Vs temperature and (4) Hall mobility. The structural characterization will involve (1) Precise single crystal and powder X-ray data collection (2) Structural analysis of the single crystal with respect to the doping concentration (3) Electron density distribution (4) Multipole structural refinements (both for single crystal and powder X-ray data) (5) Rietveld analysis of the structure using Fullprof, JANA 2000 etc. (6) Local structural analysis using the Pair Distribution Function