

Research Title Study on Thermoelectric Properties of PbTe
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Abstract

This research project has been objectives to calculate the electrical properties, thermal properties and measured the thermoelectric properties of PbTe. The $Pb_{13}Te_{14}$ cluster atom model was designed by DV-X α program to calculate orbital energy, energy gap and Fermi energy of PbTe. The super cluster atom size $4 \times 4 \times 4$ by unit cell composed of anions-256 and cations-256 to calculate the relationship of temperature and lattice parameter, elasticity, linear thermal expansion, heat capacity, thermal conductivity and electrical conductivity of PbS, PbSe, PbTe and CdTe. The electrical resistivity, Seebeck coefficient, thermal conductivity and dimensionless figure of merit of PbTe were measured and evaluated. It results show that, the PbTe crystal structure of face centered cubic, Pb5d, Pb6s, Pb6p, Te4d, Te5s and Te5p orbitals, the energy gap of 2.28 eV, Fermi energy of 0.97 eV and n-type thermoelectric material.

PbS, PbSe, PbTe and CdTe have been the lattice parameter and bulk modulus corresponding well with J. E. Ni et al. (exp.) and F. Ren et al. The bulk modulus was decreased with increasing temperature at volume and pressure constant. The shear modulus and Young's modulus were decreased with increasing temperature corresponding well with experimental. The linear thermal expansion was tendency increased corresponding well with experimental. The heat capacity was corresponded with Y. Bencherif et al. (2011) report at pressure constant. The phonon or lattice thermal conductivity, $\kappa_L(T)$ was decreased with increasing temperature which the reaction of phonon-phonon interaction (Umklapp process) at high temperature. The electrical conductivity was decreased with increasing temperature indicate that semiconductor behavior.

PbTe has been the mean density of 8.12 g/cm^3 and Vickers hardness of 35.36 HV

The relationship between thermoelectric properties and temperature together with Y.L. Pei *et al.* (2012) report were compared. The electrical resistivity of $3.1 \text{ m}\Omega\text{-cm}$ and tendency increased with increasing temperature, Seebeck coefficient of $-194.85 \text{ }\mu\text{V K}^{-1}$ indicate n-type semiconductor and tendency decreased with increasing temperature, thermal conductivity of $0.49 \text{ W m}^{-1} \text{ K}^{-1}$ more than report and

dimensionless figure of merit of 2.50×10^{-4} tendency decreased with increasing temperature and less than report.