

Theoretical Study of the Structural and Elastic Properties of Semiconducting Rare Earth Chalcogenide $\text{Sm}_{1-x}\text{Eu}_x\text{S}$ under Pressure

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Abstract : We have investigated the phase transition pressure and associated volume collapse in $\text{Sm}_{1-x}\text{Eu}_x\text{S}$ alloy ($0 \leq x \leq 1$) which shows transition from discontinuous to continuous as x is reduced. The calculated results from present approach are in good agreement with experimental data available for the end point members ($x=0$ and $x=1$). The results for the alloy counter parts are also in fair agreement with experimental data generated from the Vegard's law. An improved interaction potential model has been developed which includes coulomb, three body interaction, polarizability effect and overlap repulsive interaction operative up to second neighbor ions. It is found that the inclusion of polarizability effect has improved our results.

Keywords : elastic constants, high pressure, phase transition, rare earth compound

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