Theoretical Analysis of Semiconducting Sm$_{1-x}$Eu$_x$S under Pressure

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ABSTRACT
We have investigated the phase transition pressure and associated volume collapse in Sm$_{1-x}$Eu$_x$S alloy (0≤x≤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
High Pressure, Phase Transition, Volume Collapse, Elastic Properties, Rare Earth compound and Alloy.

1. INTRODUCTION
The studies of rare earth chalcogenides have received much attention because of their interesting properties and technological applications. They crystallize in the NaCl type structure and are semiconducting if the rare earth ion is in the divalent state and metallic if in trivalent state [1]. The divalent Eu, Sm and Yb are semiconducting and ionic in nature [2]. Jayaraman et al. [3] reported that samarium monochalcogenides undergo a pressure induced semiconductor to metal transition which is followed by a valence change of the Sm ions. The phase transition phenomena and structure stability in samarium monochalcogenides have been studied by many physicists [3-4]. Bihan et al. [4] reported that SmS shows a isostructure (Sm$^{2+}$ ion to Sm$^{3+}$) phase transition at low pressure (1.8 GPa) and after that at 42 GPa transform to CsCl. Samarium monochalcogenides are suitable for industrial and technological applications especially in pressure sensor, thermoelectric power converters, spintronics and spin filtering devices [5, 6]. One of the easiest ways to change artificially the electronic and optical properties of semiconductors is by forming their alloys. It is possible to combine two different compounds with different compounds with different optical band gaps and different rigidities in order to obtain a new material with intermediate properties.

We are motivated by the above-mentioned technological application and understanding physical properties on the effect of substitution of Eu for Sm in SmS as well as the effect of concentration and pressure on this compound and its alloy part is less studied. In the present study, we applied an improved interaction potential [7] model (which includes polarizability effect) for the prediction of phase-transition pressures, associated volume collapses and elastic module of Sm based alloy. These properties have been calculated by using Vegard’s law.

2. METHOD OF COMPUTATION
The application of pressure on the crystals causes the decrease in their volume which, in turn leads to an increased charge transfer arising due to occurrence of the deformed (or exchange) charge between the overlapping electron shells of the adjacent ions. These transferred charges interact with other distant charges via Coulomb force and give rise to many body interactions (MBI) [8]. The stability of a particular structure is always decided by the minima of the Gibbs free energy (GeU+PV-TS). Here U is the internal energy at 0K which corresponds to the cohesive energy and S is the vibrational entropy at absolute T, Pressure P and volume V. The Gibbs free energies for NaCl and CsCl structures at 0K are given by [4]:

\[
G_{B1}(r') = U_B(r') + PV_B(r')
\]

\[
G_{B2}(r') = U_B(r') + PV_B(r')
\]

Where

\[
U_B(r) = -\frac{\alpha \mu Z^2 e^2}{r} - \frac{12 \alpha \mu Z e^2}{r} \frac{f(r)}{2^2} - \frac{e^2(a_i + a_f)}{2^2}
\]

\[
+ 6b\beta_2 \exp[(r_i + r_j - r)/\rho] + 6b\beta_2 \exp[(2r_i - 1.414r)/\rho]
\]

\[
+ 6b\beta_2 \exp[(2r_j - 1.414r)/\rho]
\]

\[
U_B(r) = -\frac{\alpha \mu Z^2 e^2}{r} - \frac{16 \alpha \mu Z e^2}{r} \frac{f(r)}{2^2} - \frac{e^2(a_i + a_f)}{2^2}
\]

\[
+ 8b\beta_2 \exp[(r_i + r_j - r)/\rho] + 3b\beta_2 \exp[(2r_i - 1.514r)/\rho]
\]

\[
+ 3b\beta_2 \exp[(2r_j - 1.154r)/\rho]
\]

Here $V_{B1} = (2 \times r^3)$ and $V_{B2} = (1.54 \times r^3)$ are the unit cell volumes for B1 and B2 structures respectively. The first term in the above equation represents the lattice energies for B1 and B2 structure. These energies contain only three model parameter whose values have been determined from the knowledge of the first and second order derivatives of lattice energy which have been reported in our earlier work [7].

The mixed crystals, according to the virtual crystal approximation (VCA) [9], are regarded as an array of average ions whose masses, force constants, and effective charges are
considered to scale linearly with concentration \(x\). The measured data on lattice constants in Sm\(_{1-x}\)Eu\(_x\)S [10] have shown that they vary linearly with the composition \(x\) and hence they follow the Vegard’s law:

\[
a(AB_xC_{1-x}) = (1-x)a(AB) + xa(AC) \quad (3)
\]

The method of evaluation of three model parameters of endpoint members is the same as given in [7]. The values of these model parameters for their mixed crystal components have been determined from the application of Vegard’s law to the corresponding measured data for AC (SmS) and BC (EuS).

### 3. RESULT AND DISCUSSION

For the study structural and elastic behavior of this alloy we have calculated the model parameters. The method for calculations of transition pressure and second order elastic constants are same which we have reported in our earlier work [7]. To know the relation of transition pressure with composition, we have plotted the variation of transition pressures with composition \(x\) in Figure 1 and compared with experimental values. The results of the lattice model calculations yield the phase transition pressure of 42 (SmS) 36.87 (Sm\(_{0.75}\)Eu\(_{0.25}\)S), 31.75 (Sm\(_{0.5}\)Eu\(_{0.5}\)S), 26.63 (Sm\(_{0.25}\)Eu\(_{0.75}\)S) and 21.1 (EuS) GPa respectively. For all these compounds excellent agreement is founds with available data on the phase transition pressure.

Table 1. Model parameters for Sm\(_{1-x}\)Eu\(_x\)S

<table>
<thead>
<tr>
<th>Crystal</th>
<th>(b)</th>
<th>(\rho)</th>
<th>(f(r))</th>
</tr>
</thead>
<tbody>
<tr>
<td>SmS</td>
<td>0.483</td>
<td>0.278</td>
<td>-0.0066</td>
</tr>
<tr>
<td>Sm(<em>{0.75})Eu(</em>{0.25})S</td>
<td>0.439</td>
<td>0.266</td>
<td>-0.0068</td>
</tr>
<tr>
<td>Sm(<em>{0.5})Eu(</em>{0.5})S</td>
<td>0.394</td>
<td>0.254</td>
<td>-0.0069</td>
</tr>
<tr>
<td>Sm(<em>{0.25})Eu(</em>{0.75})S</td>
<td>0.350</td>
<td>0.242</td>
<td>-0.0071</td>
</tr>
<tr>
<td>EuS</td>
<td>0.306</td>
<td>0.230</td>
<td>-0.0073</td>
</tr>
</tbody>
</table>

### 4. FIGURES

Fig 1: The variation of transition Pressure with concentration \(x\).

Fig. 2 Variation of elastic module with concentration \(x\).
5. CONCLUSION
As improved interaction potential model is formulated in analyzing the structural as well as elastic properties in Sm$_{1-x}$Eu$_x$S. This is one of the semiconductor alloy which are solid solutions of two or more semiconducting elements, have important technological applications, especially in magnetic semiconductors industrially, e.g. in the form of fast light beam addressable memory systems in computers, as magneto-optical modulators or as magnetic field activated electronic switches and have a lot of future scopes also. At ambient pressure the semiconducting Sm$_{1-x}$Eu$_x$S alloy crystallize in a B1(NaCl) structure. As pressure is raised, these semiconducting alloy show the B1 to B2 structural phase transitions. The obtained values of material parameters allow us to predict the phase transition pressure.

The calculated value of second order elastic constants $C_{11}$ and $C_{12}$ increase with increase in pressure up to the phase transition pressure that identifies the high pressure structural stability of Sm$_{1-x}$Eu$_x$S compounds. Further, $C_{44}$ decrease linearly with the increase of pressure and does not tend to zero at the phase transition pressures and is in accordance with the first order character of the transition.

6. ACKNOWLEDGMENT
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7. REFERENCES