Mechanical Properties of a class of Magnetic Semiconductors under high pressure Engineering Applications

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Abstract—The pressure dependent ductile (brittle) nature of europium monochalcogenides compound is computed by formulating an effective interionic interaction potential consisting the long-range Coulomb, the Hafemeister and Flygare type short-range overlap repulsion extended upto the second neighbor ions and the van der Waals (vdW) interaction. From the elastic constants the Poisson's ratio ν, ratio $R_{G/B}$ of G (Voigt averaged shear modulus) over B (bulk modulus) are calculated. It is noticed that EuX (X = O, S, Se, Te) monochalcogenides are brittle at low pressures in B1 phase and ductile in B2 phase after the transition pressure.

Index Terms— Alloys, Pressure effects, Ductility, Mechanical properties *(key words)*
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I. INTRODUCTION AND REVIEW

A class of semiconductors used in mechanical engineering applications of magneto modulators and optic memories. These are known as Europium chalcogenides (EuX: X = O, Se, S and Te) and are the rare earth compounds crystallizing in rock salt structure and are, in general, magnetic semi-conductors. These technologically important compounds are semiconducting, if the rare-earth (Eu) ion is in the divalent state and metallic if it is in trivalent state [1–2], due to 4f electron promotion into the 5d conduction band states [3,4]. It is found that this 4f electron promotion is due to the decrease in energy separation between the localized 4f electronic state and 5d conduction band states with the increase in pressure [3, 4]. X-ray diffraction (XRD) and neutron-scattering studies show that under normal conditions EuX compounds crystallize in the NaCl-type structure and the lattice parameter a decreases when X moves from Te to O. [3,4].

The applied pressure plays a very vital role in chaging the structure. The structural phase transition pressures for EuO, EuS, EuSe and EuTe are 40 GPa, 21.5 GPa, 14.5 GPa and 11 GPa, respectively [2]. Europium oxide is the only Eu chalcogenides that shows an isostructural transition near 30 GPa and the NaCl to CsCl type transition near 40 GPa. EuSe, like most of the other rare earth-mono chalcogenides, undergoes a phase transformation from NaCl-type (B1) to CsCl-type (B2) structure at about 14.5 GPa [4].

Motivated from the available information on structural phase transition, we intended to seek the role of pressure dependent brittle (ductile) nature in NaCl-type (B1) to CsCl-type (B2) structure in EuX (X = O, S, Se, Te). To our knowledge this is the first quantitative theoretical prediction of the ductile (brittle) nature of Europium monochalcogenides and still awaits experimental confirmations.

II. THE GIBB'S FREE ENERGY

WThe stability of a particular structure is decided by the minima of Gibbs's free energy, $G = U + PV – TS$, U being the internal energy, which at $T = 0$ K corresponds to the cohesive energy, S is the entropy at absolute temperature T, pressure P and volume V. The Gibbs's free energies

$$G_{B1}(r) = U_{B1}(r) + PV_{B1} \qquad \text{a)}$$

$$G_{B2}(r^{'}) = U_{B2}(r^{'}) + PV_{B2} \qquad \text{b)}$$

at $T = 0$ K for *B1* phase and *B2* phase become equal at the phase-transition pressure *P*. Here, r (r') being the nearest-neighbour distance for *B1* (*B2*) phase. The notations $U_{B1}(r)$ [$U_{B2}(r')$] denotes cohesive energies for *B1* [*B2*] phases.Details of the method of calculation for cohesive energies, elastic and high-pressure properties are reported elsewherec.

III. RESULTS AND DISCUSSIONS

The ductility and brittleness of rare earth compounds europium monochalcogenides are important and can be known from second order elastic constants. We have deduced the values of free parameters modified ionic charge (Z_m), range (ρ) and hardness (*b*) from the knowledge of equilibrium distance and the bulk modulus [5]. While estimating these values we have used the input parameters for EuX: (X = O, Se, S and Te) as r_0 = 2.57, 2.985, 3.096, and 3.30 (in units of 10^{-8} cm), [4] and B_T = 110,61,52,40 GPa [4]. We have then estimated the materials parameter of EuX: (X = O, Se, S and Te) as *b* = 2.183, 4.752, 7.977, and 10.84 (in units of 10^{-12} erg,) ρ =2.83,3.23,3.34 and 3.53 (in units of 10^{-9} cm). By calculating the ratio $R_{G/B}$ [6] of Voigt averaged shear modulus *G* and the bulk modulus *B* and the Poisson's ratio [7] we can determine its ductile (brittle) behaviour.

If $R_{G/B}$ < 0.5, the material behaves in a ductile manner, otherwise the material behaves in a brittle manner and, the Poisson's ratio is less than 0.33 for brittle materials otherwise the material behaves in a ductile manner

From Figure I the ratio $R_{G/B}$ and the Poisson's ratio show the brittle nature in NaCl (B1 phase) and ductile nature in CsCl (B2 phase).

Through the calculated elastic constants, we can obtain the other mechanical properties such as elastic anisotropy at various pressures for Eu*X* compounds
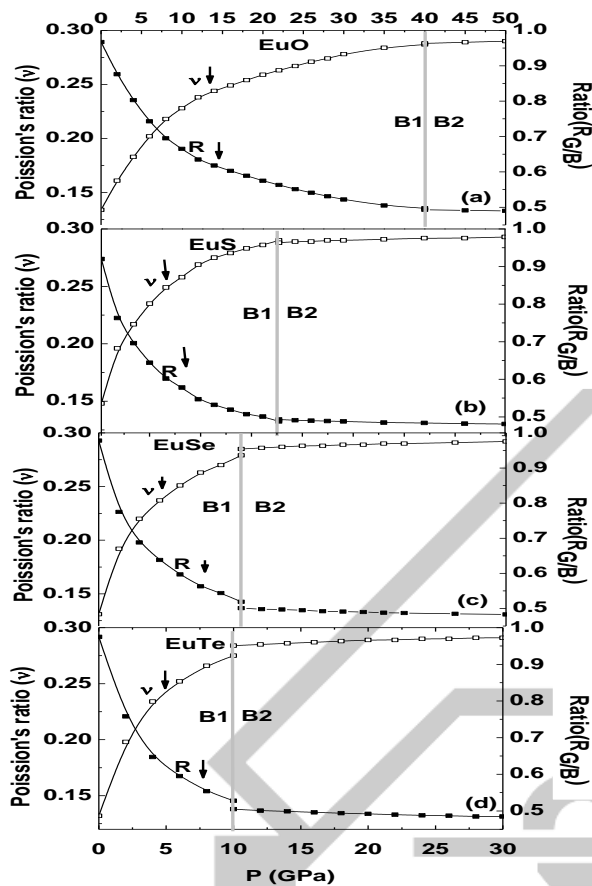

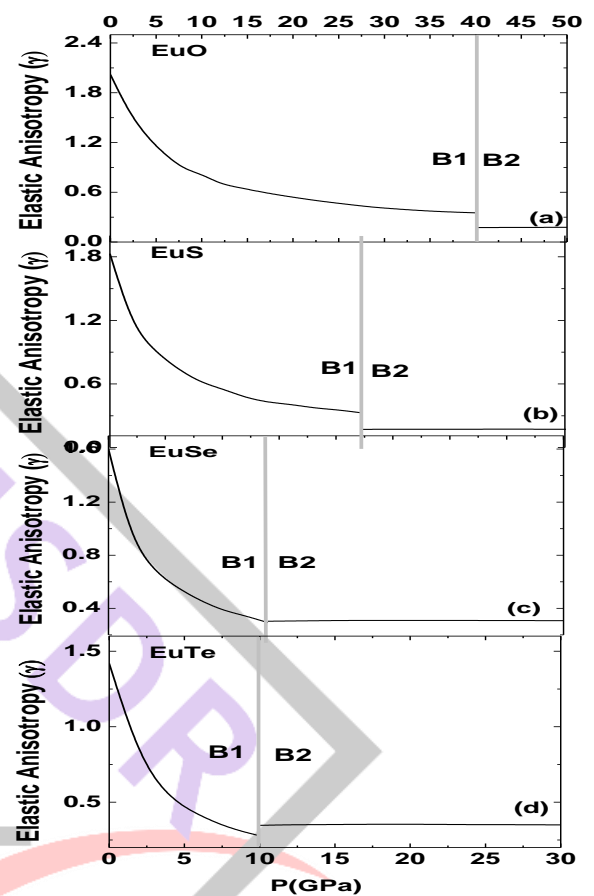**Figure 1.** Variation of Poisson's ratio ν and ratio $R_{G/B}$ with pressure

Figure 2. Variation of anisotropic (*γ*) with pressure. It is clear from Figure II   that Eu*X* (X = O, S, Se, Te) are elastically anisotropic compounds

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