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PHONON DENSITY OF STATES OF EUROPIUM SELENIDE UNDER PRESSURE

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Abstract
A remarkable feature observed in EuSe is that, it exhibits various magnetic phases with changing temperature; it is antiferromagnet II at temperature between 0-1.8K, ferri between 1.8-2.8 K and antiferromagnetic I between 2.8-4.6 K. Such magnetic behavior in EuSe is attributed to the change in lattice constant. Thus application of pressure to this compound can be very interesting through the decrease in lattice constant. In the present investigation one phonon density of states of Europium selenide have been calculated under pressure by using a simple lattice dynamical theory namely the three body force rigid ion model (TRIM) which includes long range three body interactions arising due to charge transfer effects. We have observed a pronounced shift in phonon spectrum to the higher frequency side as pressure is increased.

Key-words: Phonon, Model, Pressure

Introduction

The Europium selenide is a rare earth (RE) compounds crystallizing in rock salt structure and in general, is a magnetic semiconductor. The main interest in Eu chalcogenides compounds is in their possible application in magneto-optic memories and modulators. Also much of the interest was shown in these materials in increasing the magnetic ordering temperature, with room temperature as final goal, to make the practical applications of Eu-chalcogenides realistic [1]. Recently, III –V compound semiconductors have been randomly substituted by Eu ions, which leads to appearance of several interesting properties in these semiconducting materials some of which are well suite for device application. In a recent study Hatano et.al [2] have measured the Raman spectra of Eu under hydrostatic pressure up to 2.1 GPa by using a diamond anvil cell method.

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Model Theory

In order to describe the phonon dispersion curves of Europium chalcogenides, we use a three body force rigid ion model, already discussed by Singh [3]. In the present model, we consider the many body interactions to arise from the nearest neighbor ions. The dynamical matrix corresponding to TRIM can be written as [4]

$$D(q) = R + Z_m(C + T)Z_m \quad (1)$$

where R and C the repulsive and Coulomb matrices. T is three body force interaction matrix and Zm is matrimodified ionic charge, defined as,

$$Z_{me} = +Ze[1 + 2nfr(z)] \quad (2)$$

where f(r) is the TBI parameter, signifying the amount of overlap

The present model has seven parameters which are obtained from macroscopic quantities (e.g., elastic constants, zone centre and zone boundary frequencies). The equations relating to the macroscopic properties with the model parameter are already available in literature [4]. Input constants used to calculate the model parameter for EuSe area taken from references [5-7]. Calculated model parameters are presented in Table I.

Phonon Density of States

Several efforts have been made to understand the optical properties of Eu- chalcogenides at extreme condition such as increase in pressure or temperature. Even at ambient temperature these materials have large amount of point defect. At ambient conditions it undergoes a phase transition to the rocksalt phase near 13 GPa [8]. This fact leads to spin-disorder and the first order Raman spectra resembles to one phonon density of states. The calculated phonon DOS closely agree with the experimental data except a peak at 37 meV. The calculated phonon dispersion relations are also compared with those of the bulk phonons and anomalous behavior is discussed in detail [9]. In the present paper we have calculated the one phonon density of states (OPDS) close to the phase transition pressure for EuSe using three body force rigid ion model (TRIM). Since there is no experimental measurements available except at very low pressure up to 2.1 GPa [2], we could not compare all the OPDS at pressure above 2 GPa. However there is good agreement between the experimental Raman measurements of Hatano et.al [2] with OPDS obtained from present calculation, which has been presented in fig. [1(b)]. The peak G measured by Hatano et.al [2] at high pressure (up to 2.1 GPa) is correctly predicted in the present calculation of one phonon density of states for EuSe.

In fig.2, we have presented the calculated one phonon density of states for EuSe at different pressure close to its phase transition. It is evident from this figure that as the pressure is increased there is a remarkable shift in the peak position towards higher frequency side.

Finally, in the present paper, we have reported the calculated result on density of states for EuSe at different pressure using a lattice dynamical model theory namely the three body force rigid ion model. The calculated result are in food agreement with the available experimental observation, reported so for.

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Table I: calculated model parameter for EuSe

Parameter	1 atm	12.0 GPa
A_{12}	19.48	26.5476
B_{12}	-2.000	-4.6315
A_{11}	-0.1132	-0.1307
B_{11}	0.0119	0.0096
A_{22}	1.171	6.5962
B_{22}	-0.620	-1.632
Z_m	1.32	1.30

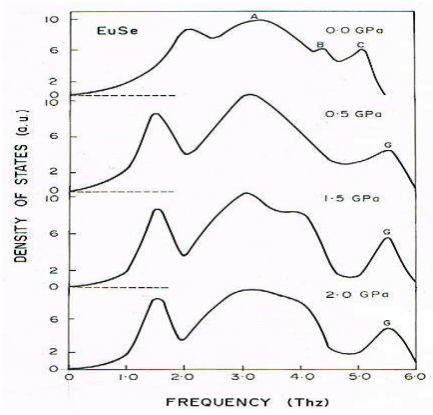

Fig. 1 (a): One phonon density of states close to the phase transition pressure for EuSe

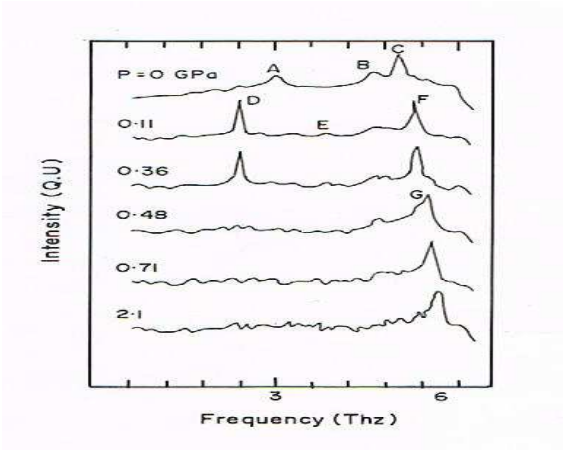

Fig. 1(b): One phonon density of states close to the phase transition pressure for EuSe

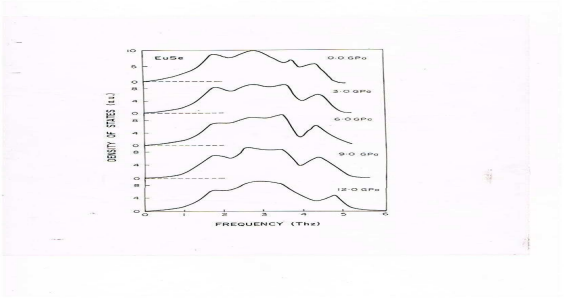

Fig. 2