Lattice Dynamical Study and Elastic Property of Europium Telluride (EuTe) Crystal

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ABSTRACT

In the present work authors are reporting complete lattice dynamical properties of Europium telluride (EuTe). The present model works on three body rigid ion model & three body rigid shell model (TRIM & TRSM). The short-range overlap repulsion is operative up to the second neighboring ions. An excellent agreement has been obtained between theory and experiment for their all-phonon properties of (EuTe) like phonon dispersion curves, Debye temperature variations, two-phonon IR/Raman spectra, third-fourth order lattice constant, pressure derivative and anharmonic elastic properties.

Keywords: Phonon dispersion curves, Debye temperature variations, Two-phonon IR/Raman spectra, Third-fourth order lattice constant, Pressure derivative, Anharmonic elastic properties.

INTRODUCTION

The electronic structure of Europium telluride (EuTe), which is a family of Europium Chalcogenides crystallize in F.C.C. NaCl structure and are also called rare earth europium chalcogenides. Europium Telluride (EuTe) is a crystal grown product generally immediately available in most volumes. Unlike other rare earth compounds europium chalcogenides generally, show non-mixed valance character. Complete experimental data on phonon dispersion is available for EuTe, which has been reported. by Silberstein et al.,1. Zeyher and Kress2 discuss the complete phonon dispersion curves (PDC), combined density of states (CDS)3 and Debye temperature variations curve given by4. The parameters like elastic & dielectric constants5,6, the physical-natural properties of the (EuTe) have been attracted and their explication through different conceptual models7-12, which has also satisfyingly narrated their engrossing properties. It has been establishing the interactions of three body which demonstrate the optical branches and Cauchy discrepancy concurrently to almost all the ionic-semiconducting crystals13. The remarkable success achieved from (RIM)14 and (RSM)15 represent the lattice properties of alkali halides and worthwhile to explore the adequacies of these model for EuTe. The third-order elastic constants (TOEC), which is related to the energy products of three strain
components, and the lowest order constants to enter the description of non-linear effects like the equation of state and the interaction of phonons. These TOEC is determined from velocity measurements on small amplitude sound waves in statically stressed media. The aim of present report is to test the applicability and utility of second-neighbor three-body rigid shell model (TRSM) and second neighbor three-body rigid ion model (TRIM) with the satisfactory description of phonon dispersion relations and other phonon properties of the EuTe.

Theory

The existing model accordingly consists of the comprehensive shield coulomb, TBI and the short-range overrun repulsion effective up to the next-neighbor for EuTe. The relevant expression for the crystal potential per unit cell can be extrapolate TBFSM, is given as

$$\Phi = \Phi^C + \Phi^R + \Phi^{TBI}$$  \hspace{1cm} (1)

where $\Phi^C$ is comprehensive Coulomb reciprocity potential. where $\Phi^R$ is a short-range repulsion & $\Phi^{TBI}$ long-range TBI interaction potential by16. The secular determinant equation is given by:

$$\left[ \frac{2}{\omega^2} - \frac{M_L}{M_J} \right] = 0$$  \hspace{1cm} (2)

The dipole's (VWI) efficient next-neighbor is given as:

$$\Phi_{\text{VWI}}^{(r)} \left( r \right) = -S \frac{C_{++} + C_{-+}}{6r^5} = \Phi^{V} \left( r \right)$$  \hspace{1cm} (3)

By use of Eq. (2) the Eq. for elastic constants can give as:

$$C_{ij} = \frac{\gamma^2}{4\eta^2} \left[ 5.1112 Z_{ij} + A_{ij} + \frac{1}{2} \left( A_{ij} + A_{ji} \right) + \frac{1}{2} \left( A_{ij} + A_{ji} \right) \right] - 9.3204 \frac{\gamma^2}{4\eta^2} \left[ 5.1112 Z_{ij} + A_{ij} + \frac{1}{2} \left( A_{ij} + A_{ji} \right) + \frac{1}{2} \left( A_{ij} + A_{ji} \right) \right]$$  \hspace{1cm} (4)

$$C_{12} = \frac{\gamma^2}{4\eta^2} \left[ 0.226 Z_{12} + B_{12} + \frac{1}{2} \left( A_{12} + A_{21} \right) - \frac{1}{4} \left( A_{12} + A_{21} \right) + 9.3204 \frac{\gamma^2}{4\eta^2} \left[ 0.226 Z_{12} + B_{12} + \frac{1}{2} \left( A_{12} + A_{21} \right) - \frac{1}{4} \left( A_{12} + A_{21} \right) \right]$$  \hspace{1cm} (5)

$$C_{44} = \frac{\gamma^2}{4\eta^2} \left[ 2.555 Z_{44} + B_{44} + \frac{1}{4} \left( A_{44} + A_{44} \right) + \frac{3}{4} \left( A_{44} + A_{44} \right) + 9.3204 \frac{\gamma^2}{4\eta^2} \left[ 2.555 Z_{44} + B_{44} + \frac{1}{4} \left( A_{44} + A_{44} \right) + \frac{3}{4} \left( A_{44} + A_{44} \right) \right]$$  \hspace{1cm} (6)

Vibrational Properties of EuTe

The term $f_0$ is based on overlap integrals of charge ($e$) wave functions and expressions for optical vibration frequencies ($\omega_1$ and $\omega_2$) are given as:

$$\left( \mu_a \omega_{L}^2 \right)_{\eta=0} = R_0 + \frac{\left( Z \omega \right)^2}{\sqrt{f_L}} \left[ -\frac{2\pi}{3} \left( Z \omega \right)^2 + 6 \left( Z \omega \right)^2 \right]$$  \hspace{1cm} (7)

$$\left( \mu_a \omega_{T}^2 \right)_{\eta=0} = R_0 - \frac{Z \omega}{\sqrt{f_T}} \cdot \frac{4\pi}{3} \left( Z \omega \right)^2$$  \hspace{1cm} (8)

By using Debye’s model distribution function for frequency is given by

$$\Theta_0 = h \nu_0 / K$$  \hspace{1cm} (9)

the density of states of phonon for each polarization is given by

$$g (\omega) = \frac{dN}{d\omega} = N \int_{\Theta} \frac{d\omega - \omega}{g} (\omega) = (VK^3/\omega \delta \omega) dK / d\omega$$  \hspace{1cm} (10)

and $N = (L/2\pi)^3 (4\pi K^3/3)$ and phonon wave vector $q$ such that $\int g (\omega) d\omega = 1$

Numerical computations

The input data and calculated model parameters from SMTRSM and SNTRIM for EuTe are given in Table 2.

| Table 1: Cauchy-Discrepancy (in units $10^{12}$ dyne/cm²) for EuTe |
|---|---|
| Property | Values for EuTe |
| $C_{11} - C_{44}$ | -0.3501831 |
| $C_{12} - C_{44}$ | 0.2610215 |
| $C_{14} - C_{44}$ | 0.0870346 |
| $C_{11} + C_{12}$ | 0.01739689 |
| $C_{11} + C_{14}$ | 2.3062965 |
| $C_{11} + C_{15}$ | 0.1261647 |
| $C_{11} + C_{16}$ | 0.637605 |
| $C_{11} + C_{17}$ | -0.0232144 |
| $C_{11} + C_{18}$ | -0.1482605 |
| $C_{11} + C_{19}$ | -0.4385078 |
| $C_{11} + C_{20}$ | -0.4158073 |

| Table 2: Input data, model parameters for EuTe in- $C_i$ (in $10^{12}$ dyn/cm²), ro(in $10^{-8}$ cm) |
|---|---|---|---|
| Input data for EuTe | Model parameters for EuTe |
| Properties | Values for EuTe | Parameters | TRSM | TRIM |
| $\tau_{11}$ | 9.36 | $Z_{11}$ | 0.67 | 0.5965 | 0.5722 |
| $\tau_{12}$ | 1.63 | $Z_{12}$ | 0.24 | -0.6950 | -0.6667 |
| $\tau_{13}$ | 8.76 | $d_{1}$ | 3.292 | 0.4136 | 0.9680 |
| $\tau_{14}$ | 3.96 | $d_{2}$ | 0.9680 | 0.4136 | 0.9680 |
| $\tau_{15}$ | 8.76 | $Y_{1}$ | -0.2382 | -0.4385078 | -0.4158073 |
| $\tau_{16}$ | 3.292 | $Y_{2}$ | -3.7420 | -0.4158073 | -0.4158073 |
Table 3: Combined Density States curve for EuTe

| Raman Active-(Present study) | Branch       | Values (cm⁻¹) |
|-----------------------------|--------------|---------------|
|                             | L₀(X)−Lₐ(Δ)  | 43            |
|                             | L₀(X)−Tₐ(X)  | 75            |
|                             | Lₐ+Tₐ(X)     | 118           |
|                             | Lₐ(X)+Tₐ(Δ)  | 158           |
|                             | 2Lₐ(Δ)       | 172           |
|                             | Tₐ+Lₐ(Δ)     | 189           |
|                             | 2T₀(Δ)       | 205           |
|                             | 2L₀(X)       | 233           |
|                             | 2L₀(Δ)       | 255           |
|                             | 2L₀(↑)       | 286           |

Table 4: TOEC & FOEC (in units 10¹² dyne/ Cm²), Pressure derivatives of SOEC and TOEC for EuTe

| TOEC and FOEC (in units 10¹² dyne/Cm²) | Pressure derivatives of SOEC and TOEC (dimensionless) |
|-----------------------------------------|-------------------------------------------------------|
| Property EuTe (Present)                | Property EuTe (Present)                              |
|-----------------------------------------|-------------------------------------------------------|
| C₁₁₁                                    | dK'/dP 66.328857                                      |
| C₁₂₂                                    | dS'/dP 36.399633                                      |
| C₁₄₄                                    | dC'₁₁₁/dP -2.7321557                                  |
| C₁₉₅                                    | dC'₁₁₂/dP -4263.2546                                  |
| C₁₆₆                                    | dC'₁₁₆/dP -3.3262317                                  |
| C₂₁₁                                    | dC'₁₂₁/dP 2.7392656                                   |
| C₂₅₃                                    | dC'₁₂₂/dP 1.6209                                      |
| C₂₅₅                                    | dC'₁₂₅/dP -1.7668426                                  |
| C₃₄₄                                    | dC'₁₃₄/dP 1.5284741                                   |
| C₃₄₅                                    | dC'₁₃₅/dP 2.0584741                                   |
| C₄₅₆                                    | dC'₁₄₆/dP -1.7668426                                  |
| C₄₄₄                                    | dC'₁₄₄/dP 2.7392656                                   |
| C₄₄₅                                    | dC'₁₄₅/dP 1.6209                                      |
| C₄₅₅                                    | dC'₁₄₆/dP -1.7668426                                  |
| C₄₄₆                                    | dC'₁₄₄/dP 2.7392656                                   |

RESULTS

The present approach is effectively described the crystal dynamics of (EuTe), eight parameter's with elastic constants (C₁₁₁, C₁₂₂ & C₄₄₄), six short range force constants parameters r₀, f₀, ⁰, ionic charge z, shell charge Y, polarizabilities (α₁, α₂) & polarizability (mechanical) ‘d’ developed by16 for (EuTe) are reported in Table 1 by using Eq.1 & 2. The knowledge of lattice vibration frequency (CDSc) reports in Table 2 by computing N (ν + ν'), the combined density data is reported in Table 3. The sensitivity of two-phonon Raman spectra is towards high-frequency side of the phonon spectra & specific heats towards its lower side is confirmed the validity of present model for its full wavelength range. The 3rd & 4th order elastic constant and its pressure derivatives for (EuTe) are given in Table 4. Which is probably the first reports in the
absence of experimental data, but their reliability test is not possible. The reported result by use of SNTRSM for (EuTe) is comparatively nearer to the measure data on PDCs, which are showing in the Fig. 1(a), (b) & (c). These results for TMC and its some features of PDC for (EuTe) are specially reporting here. The interactions of three body have affected both LO & TO branches, more than acoustic branches (LA and TA). Other striking feature is excellent reproduction of optical and acoustic branch. The model parameter of TRSM & TRIM is used to calculate the frequency along with uniformity and curve is plotted between wave vectors versus obtain (PD) from this model. These curves are measure up with use of inelastic neutron scattering technique. The specific heat data has been enumerating at variable temperature by Blackmann’s\textsuperscript{17} and the Debye temperature curve is plotted with absolute temperature (T). Qualitatively the TRSM model is prominent than some of the model values. In addition, some other researchers\textsuperscript{18-22} of the same field of research have also tried to report their best to explain PDCs and other properties of europium chalcogenides but only with moderate success. To increase the merit of this work we have calculated two phonon IR/Raman spectra and alteration of Debye temperatures shown in Fig. 2. The (CDS) peaks is compare with theoretical data, shown in Fig. 3. The interpretation of critical point study has been used by Burstein \textit{et al.},\textsuperscript{23}

**CONCLUSION**

Although, quantitively the agreement achieved from our present model TRSM is good. Furthermore, slight discrepancies still occurring between theory and experiment may be further improved by including the effect of free carrier screening (FCS), Van der Waals interactions (if data are available in future) and by including anharmonic vibrations in the present model (TRSM). A large group of researchers also have successfully reported theoretical results for some other alkali halides and semiconducting materials\textsuperscript{24-31} by use of the present model which shows the validity of this model.

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**Conflict of interest**

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