Indian Journal of Pure & Applied Physics
Vol. 62, September 2024, pp. 834-840
DOI: 10.56042/ijpap.v62i9.8072

Temperature Dependent Elastic and Ultrasonic Properties of Rare-earth Europium Monopnictides EuX(X=N, P, As, Sb)

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Received 15 January 2024; accepted 8 August 2024

The temperature dependent mechanical, thermo-physical and nonlinear ultrasonic properties of europium monopnictides EuX (X: N, P, As and Sb) were studied in this exploration. The 2[nd] and 3[rd]order elastic constants (SOECs and TOECs) of EuX were computed with the help of Coulomb and Born-Mayer potential applying two fundamental indicators *i.e.*, the nearest neighbour distance and the hardness parameter in the temperature span 100-300K. Further the SOECs are applied to enumerate the mechanical variables such as elastic moduli, Zener anisotropic ratio, Poisson's ratio and Pugh's index using Voigt-Reuss-Hill (VRH) approach at T=300K. The results derived from elastic and mechanical properties confirm the mechanical stability and brittle nature of EuX. The acoustical velocities have been enumerated using the SOECs and density of EuX along <100>, <110> and <111> directions at T=300K. All above physical parameters have been utilized to compute the direction dependent Grüneisen parameter and Debye characteristic temperature of EuX at T=300K. The achieved values of this exploration are discussed and equated with materials of similar characteristics.

Keywords: Europium monopnictides; Elastic constants; Mechanical constants; Ultrasonic grüneisen parameter

1 Introduction

Ultrasonics play vital role for the material characterization in different physical conditions. Applications of ultrasonics include non-destructive testing (NDT), medical diagnostics, measurement and evaluation of elastic properties of materials, communication devices, depth sounding, medical therapy, machining of materials, disruption of biological cell, and homogenization of materials etc.[1]. The study of ultrasonic attenuation of the substances has attained new area with the development in the engineering and material science. The investigators explained the temperature reliant part of the ultrasonic attenuation where acoustical phonons and thermal phonons interact with each other in lattice[2]. The elastic constants of the substances provide important information about the behaviour of the atomic bonding force[3]. The potential applications of rare-earth materials have been described with powerful assets in terms of the reliability, the efficiency and the longevity. The rare-earth materials have been applied in modern applications such as cameras, mobile phones, energy-efficient light bulb, computer hard drives, fiber optic lines, high intensity flood lights for stadiums and permanent magnets etc.[4]. The rare-earth monopnictides are the potential candidates of rare earth family for making spintronics devices[5]. Duan *et al*.[5] analyzed the electronic and magnetic features of number of rare-earth (RE) monopnictides including Europium monopnictide. The electronic structures of the europium chalcogenides and pnictides have been computed utilizing corrected local-spin-density approximation (SIC-LSD) by Horne *et al*.[6]. The mechanical and thermal characteristic of europium monochalcogenides were studied by Bhalla *et al*.[7]. Söllinger *et al*.[8] have investigated the exchange integrals for EuX (X= S, Te, Se, or O)by using classical Heisenberg model. Ghosh*et al*.[9] have investigated electronic structure and magnetic characteristic of europium monochalcogenides by virtue of full potential linear muffin-tin orbital process.

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Although some of rare-earth chalcogenides and pnictides have been investigated in literature[10,11] but no one has attempted ultrasonic studies on EuX. So this motivates us to explore the ultrasonic study associated with elastic properties. The main purpose of this investigation is to examine the elastic and ultrasonic features of europium monopnictides with in temperature span 100-300K along <100>, <110> and <111> orientations using the tested methods.

2 Theory

The 2nd and 3rd order elastic constants at different temperature range are assessed by sum of static part and vibrational part of elastic stiffness constant as

$$C_{ij}(T) = C_{ij}^{0} + C_{ij}^{vib} \quad \& \; C_{ijk}(T) = C_{ijk}^{0} + C_{ijk}^{vib}$$

Where the superscription '0' depicts the elastic constants at absolute zero temperature and superscription '*vib*' stands for the elastic constants at perticular temperature.

The interionic Coulomb & Born potential has obtained by sum of long range electrostatic and short range repulsive potentials[12]

$$\phi(r) = \phi_e(C) + \phi_R(B) \qquad \ldots (1)$$

Here $\phi_e(C)$ represents the Coulomb long range attractive potential and $\phi_R(B)$ represents the Born-Mayer short range repulsive potential.

$$\phi_e(C) = \pm\frac{e^2}{r_0} \text{ and } \phi_R(B) = A\exp.\frac{-r_0}{b} \qquad \ldots (2)$$

Where b = Born parameters, τ_O = nearest neighbor distance, e = electronic charge, A = strength parameter.

The static part of SOECs and TOECs at 0K has been calculated as[13]

$$\begin{Bmatrix} C_{11}^0 = \frac{3e^2}{2r_0^4}S_5^{(2)} + \frac{1}{br_0}\left(\frac{1}{r_0}+\frac{1}{b}\right)\phi(r_0) + \frac{2}{br_0}\left(\frac{1}{\sqrt{2}r_0}+\frac{1}{b}\right)\phi(\sqrt{2}r_0) \\ C_{12}^0 = C_{44}^0 = \frac{3e^2}{2r_0^4}S_5^{(1,1)} + \frac{1}{br_0}\left(\frac{1}{\sqrt{2}r_0}+\frac{1}{b}\right)\phi(\sqrt{2}r_0) \end{Bmatrix} \qquad \ldots (3)$$

$$\begin{Bmatrix} C_{111}^0 = \frac{15e^2}{2r_0^4}S_7^{(3)} - \left(\frac{3}{r_0^2}+\frac{3}{br_0}+\frac{1}{b^2}\right)\phi(r_0) \\ -\frac{1}{b}\left(\frac{3\sqrt{2}}{r_0^2}+\frac{6}{br_0}+\frac{2\sqrt{2}}{b^2}\right)\phi(\sqrt{2}r_0) \\ C_{112}^0 = C_{166}^0 = -\frac{15e^2}{2r_0^4}S_5^{(2,1)} \\ -\frac{1}{4b}\left(\frac{3\sqrt{2}}{r_0}+\frac{6}{br_0}+\frac{2\sqrt{2}}{b^2}\right)\phi(\sqrt{2}r_0) \\ C_{123}^0 = C_{144}^0 = C_{456}^0 = -\frac{15e^2}{2r_0^4}S_7^{(1,1,1)} \end{Bmatrix} \qquad \ldots (4)$$

$$\phi(r_0) = A\,exp\left(\frac{r_0}{b}\right) \text{ and } \phi(\sqrt{2}r_0) = A\,exp\left(-\frac{\sqrt{2}r_0}{b}\right)$$

The lattice sum values are

$S_3^{(1)} = -0.58252, S_5^{(2)} = -1.04622, S_3^{(1,1)} = -0.23185$

$S_7^{(3)} = -1.36852, S_7^{(2,1)} = -0.16115, S_7^{(2,1)} = -0.09045$

Vibrational SOECs and TOECs Constants C_{IJ}^{Vib} and C_{IJK}^{Vib} for B1 structure are given as[13]

$$\begin{Bmatrix} C_{11}^{Vib} = G_1^2 f^{(1,1)} + G_2 f^{(2)} \\ C_{12}^{Vib} = G_1^2 f^{(1,1)} + G_{1,1} f^{(2)} \\ C_{44}^{Vib} = G_{1,1} f^{(2)} \end{Bmatrix} \qquad \ldots (5)$$

$$\begin{Bmatrix} C_{111}^{Vib} = G_1^3 f^{(1,1,1)} + 3G_1G_2 f^{(2,1)} + G_3 f^{(3)} \\ C_{112}^{Vib} = G_1^3 f^{(1,1,1)} + G_1\left(2G_{1,1}+G_2\right) f^{(2,1)} + G_{2,1} f^{(3)} \\ C_{144}^{Vib} = G_1G_{1,1} f^{(2,1)} + G_{1,1,1} f^{(3)} \\ C_{166}^{Vib} = 3G_1G_{1,1} f^{(2,1)} + G_{2,1} f^{(3)} \\ C_{456}^{Vib} = G_{1,1,1} f^{(3)} \end{Bmatrix} \qquad \ldots (6)$$

Here,

$$\begin{Bmatrix} f^{(2)} = f^{(3)} = \frac{h\omega_0}{8r_0^3}\coth x \\ f^{(1,1)} = f^{(2,1)} = -\frac{h\omega_0}{96r_0^3}\left\{\frac{h\omega_0}{2k_BT\sinh^2 x} + \coth x\right\} \\ f^{(1,1,1)} = -\frac{h\omega_0}{384r_0^3}\left\{\frac{(h\omega_0)^2\coth x}{6(k_BT)^2\sinh^2 x} + \frac{h\omega_0\coth x}{2k_BT\sinh^2 x} + \coth x\right\} \end{Bmatrix} \qquad \ldots (7)$$

Here x $=\frac{h\omega_0}{2k_BT}$; *h* refers to Planck's constant.

Expressions for G_n are given by the following relations.

$$\begin{Bmatrix} G_1 = \left\{2\left[\begin{pmatrix} 2\rho_0 - \rho_0^2 + 2)\phi(r_0) \\ +2(\sqrt{2} + (2\rho_0 - \sqrt{2}\rho_0^2)\phi(\sqrt{2}r_0)) \end{pmatrix}\right]H\right\} \\ G_2 = \left\{2\left[\begin{pmatrix} -6\rho_0 - \rho_0^2 + \rho_0^3 - 6)\phi(r_0) \\ +(-3\sqrt{2} - 6\rho_0 - \sqrt{2}\rho_0^2 + 2\rho_0^3)\phi(\sqrt{2}r_0)) \end{pmatrix}\right]H\right\} \\ G_3 = \left\{\begin{bmatrix} 30\rho_0 + 9\rho_0^2 - \rho_0^3 - \rho_0^4 + 30)\phi(r_0) \\ +(\frac{15}{2}\sqrt{2} + 15\rho_0 + \frac{9}{2}\sqrt{2}\rho_0^2 - \rho_0^3 - \\ \sqrt{2}\rho_0^4)\phi(\sqrt{2}r_0) \end{bmatrix}H\right\} \\ G_{1,1} = \left\{\begin{bmatrix} (-6\rho_0 - \sqrt{2}\rho_0^2 + 2\rho_0^3 - 3\sqrt{2}) \\ \phi(\sqrt{2}r_0) \end{bmatrix}H\right\} \\ G_{2,1} = \left\{\begin{bmatrix} \left(\frac{15}{\sqrt{2}} + 15\rho_0 + \frac{9}{\sqrt{2}}\rho_0^2 - \rho_0^3 - \sqrt{2}\rho_0^4\right) \\ \phi(\sqrt{2}r_0) \end{bmatrix}H\right\} \\ G_{1,1,1} = 0 \end{Bmatrix} \qquad \ldots\ldots (8)$$

Here H is expressed as

$$H = \left[(\rho_0 - 2)\phi(r_0) + 2(\rho_0 - \sqrt{2}\rho_0^2)\phi(\sqrt{2}r_0))\right]^{-1} \text{and } \rho_0 = \frac{r_0}{b} \qquad \ldots (9)$$

When the symmetry of cubic crystal has been displayed to the hydrostatic pressure, the arrangement of fragment of the specific crystal structure is retained. The first order pressure derivatives (FOPDs) of SOECs for europium monopnictides are enumerated with SOECs and TOECs. The first order pressure derivatives are expressed as given below[11].

$$\left\{\begin{array}{l} \dfrac{dC_{11}}{dP} = -\left\{\dfrac{(2C_{11}+2C_{12}+C_{111}+2C_{112})}{(C_{11}+2C_{12})}\right\} \\ \dfrac{dC_{12}}{dP} = -\left\{\dfrac{(-C_{11}-C_{12}+2C_{112}+2C_{123})}{(C_{11}+2C_{12})}\right\} \\ \dfrac{dC_{44}}{dP} = -\left\{\dfrac{(C_{11}+2C_{12}+C_{44}+C_{144}+2C_{155})}{(C_{11}+2C_{12})}\right\} \end{array}\right\} \quad \ldots (10)$$

Further the mechanical variables such as shear modulus (G), Zener anisotropy ratio Z_A, bulk modulus (B), tetragonal modulus (Cs), Poisson's ratio (σ) and Pugh's ratio (G/B) are enumerated with the help of SOECs as follows[14]

$$\left\{\begin{array}{c} B = \dfrac{(C_{11}+2C_{12})}{3};\ G = \dfrac{(C_{11}-C_{12}+3C_{44})}{10} + \dfrac{2.5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})}; \\ \sigma = \dfrac{(3B-2G)}{(6B+2G)}; Z_A = \dfrac{2C_{44}}{(C_{11}-C_{12})}; C_S = \dfrac{C_{11}-C_{12}}{2} \end{array}\right\} \quad \ldots (11)$$

The ultrasonic velocities (V_L, V_S, V_D) are calculated in<100>, <110> and <111> directions at temperature regime 100-300K. Expressions to calculate ultrasonic velocities have been given as[14]

In <100> direction

$$V_L = \sqrt{(C_{11}/\rho)}; V_{S1} = V_{S2} = \sqrt{(C_{44}/\rho)}; \quad \ldots (12)$$

In <111> direction

$$V_L = \sqrt{(C_{11}+2C_{12}+4C_{44})/3\rho}; V_{S1} = V_{S2} = \sqrt{(C_{11}-C_{12}+C_{44})/3\rho} \quad \ldots (13)$$

In <110> direction

$$V_L = \sqrt{(C_{11}+C_{12}+2C_{44})/2\rho}; V_{S1} = \sqrt{C_{44}/\rho} V_{S2} \sqrt{(C_{11}-C_{12})/\rho} \quad \ldots (14)$$

The Debye average velocity (V_D) in relation to ultrasonic velocities (V_L, V_{S1}, V_{S2}) defined as

In <100> and <111> direction

$$V_D = \left[\frac{1}{3}\left\{\frac{1}{V_L^3} + \frac{2}{V_{S1}^3}\right\}\right]^{-1/3} \quad \ldots (15)$$

In <110> direction

$$V_D = \left[\frac{1}{3}\left\{\frac{1}{V_L^3} + \frac{1}{V_{S1}^3} + \frac{1}{V_{S2}^3}\right\}\right]^{-1/3} \quad \ldots (16)$$

The formula of Debye temperature θ_D is given below[14], which rely upon molecular weight M, Debye average velocity V_D, density ρ and number of atoms per unit cell n.

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi}\left(\frac{N_A \rho}{M}\right)\right]^{1/3} V_D \quad \ldots (17)$$

Here h and k_B are termed as Planck's constant and Boltzmann constant respectively.

The direction dependent ultrasonic Grüneisen parameters along different crystallographic directions are calculated by SOECs and TOECs[15].

3 Results and Discussion

The 2[nd] and 3[rd] order elastic constants were determined utilizing two fundamental variables i.e., the lattice parameter and the hardness constant with in temperature span 100-300K. We have chosen the lattice parameter (r_0) for EuN, EuP, EuAs and EuSb are 5.017 Å, 5.75 Å, 5.91Å and 6.26 Årespectivily[5] and hardness parameter (b) as 0.303 Å[16] for EuN, EuP, EuAs and EuSb materials. The investigated values of temperature reliant 2[nd] and 3[rd] order elastic constants for EuX are provided in Figs. 1-2.

The effect of temperature at elastic constants and the associated parameters are necessary to give the information about the mechanical strength of europium monopnictides at different temperature. For the computed results of SOECs and TOECs, it has been predicted that the elastic behaviour of europium monopnictides vary according to temperature. The four elastic constants (C_{11}, C_{44}, C_{112} and C_{144}) are increasing with increase in temperature and other four constant (C_{12}, C_{111}, C_{166}, and C_{123}) (are decreasing with increase in temperature. So we observed that these elastic constant are temperature sensitive. But elastic constant C_{456} is not changing with temperature due to zero vibrational energy so C_{456} is temperature insensitive. These types of characteristics have been already inspected in existing literature[17]. The values of

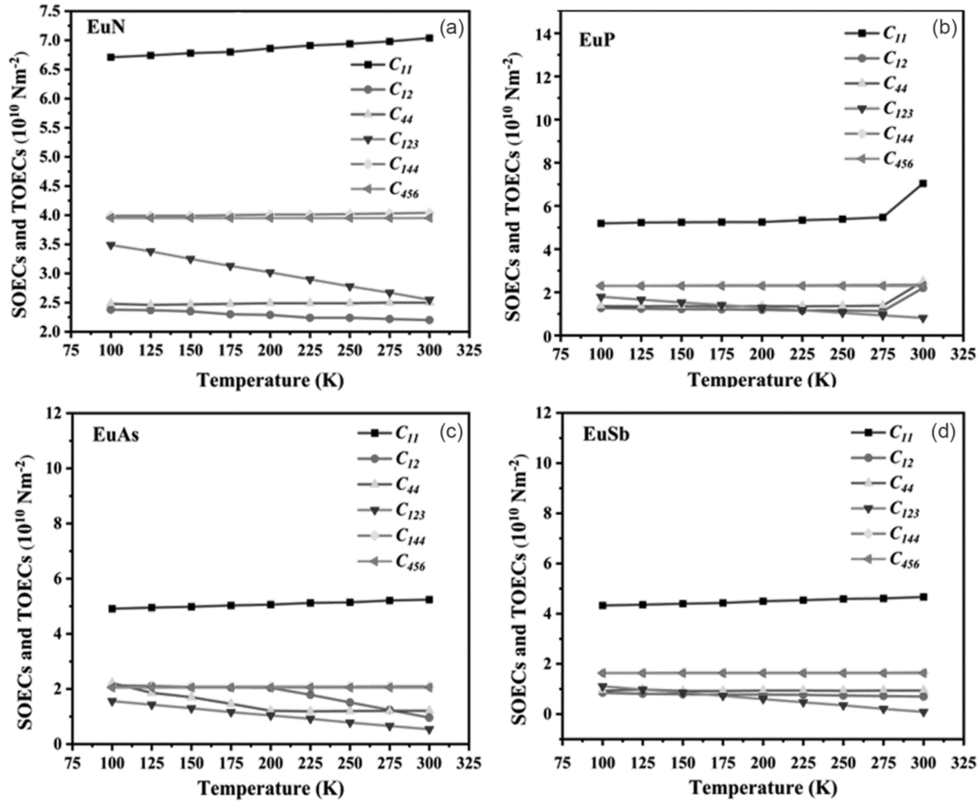

Fig. 1 — SOECs and TOECs with positive temperature gradient for (a) EuN (b) EuP (c) EuAs (d) EuSb

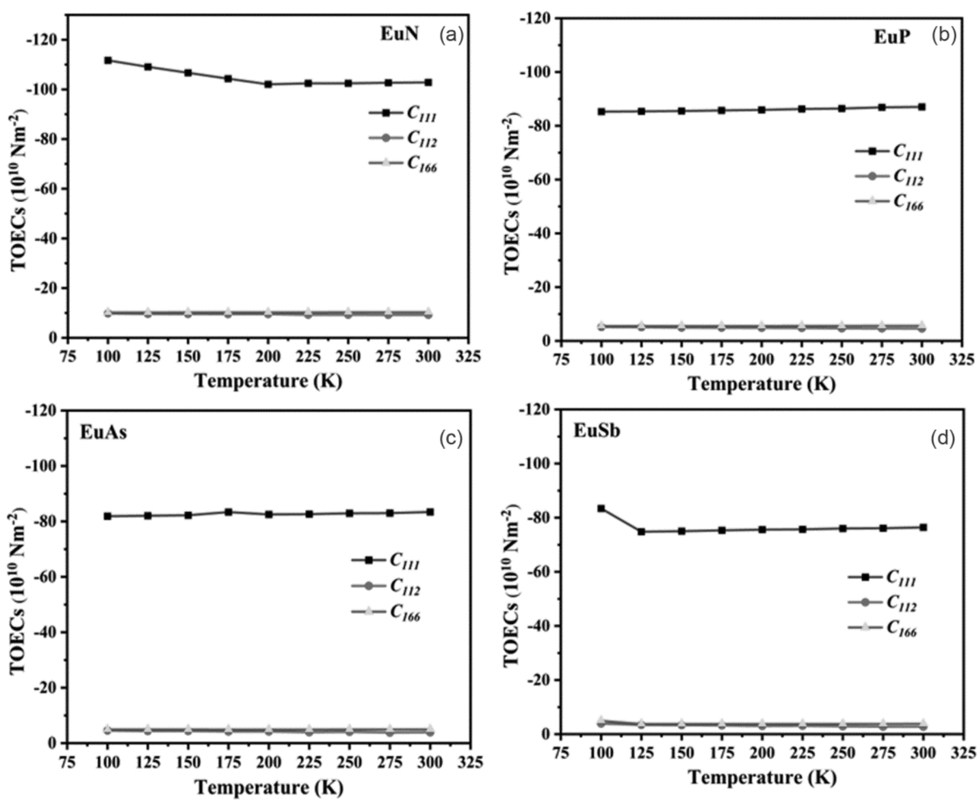

Fig. 2 — TOECs with negative temperature gradient for (a) EuN (b) EuP (c) EuAs (d) EuSb

C_{11} for EuN are highest which indicates EuN are more mechanically stable than other chosencompounds. The values of shear elastic constants C_{44} for EuN are dominating over all chosen materials which predict that EuN are harder and stiffer. Europium monopnictides fulfill the conditions of Born stability criterion[13,14], which is defined as (C_{11}+2 C_{12})/3>0, C_S= (C_{11} - C_{12})/2 > 0, C_{44}> 0 so the europium monopnictides are stable in nature.

The first order pressure derivatives (FOPDs) for SOEC were computed by using the investigated value of SOECs and TOECs in Eq. (10) for europium monopnictides. The estimated magnitude of FOPDsof SOECs is presented in Table 1.

The investigated FOPDs of SOECs determine the an harmonic properties, stiffness, softness and nature of interionic forces. The FOPDs of C_{11} *i.e.*, (dC_{11}/dP) are greater than the FOPDs of C_{12} and C_{44}. The positive pressure derivatives indicate increasing hydrostatic pressure while negative pressure derivatives indicate the decreasing hydrostatic pressure[11]. The pressure derivatives of $C_{11}$and $C_{12}$are positive for EuX while pressure derivatives of C_{44} are negative except EuN.

The enumerated results of SOECs are useful to find out the mechanical parameters like Poisson's ratio (σ), bulk modulus (B), Zener anisotropy indicator (Z_A), shear modulus (G), tetragonal modulus (Cs) and Pugh's ratio (G/B). The numerical results of $B, G, Cs, \sigma, Z_A, G/B$ are given in Table 2.

Table 1— FOPDs of SOECs for EuX (X= N, P, As and Sb) in the temperature span 100-300K

Materials	FOPDs	100K	200K	300K
	dC_{11}/dP	8.98	8.97	8.96
EuN	dC_{12}/dP	2.29	2.20	2.19
	dC_{44}/dP	0.21	0.21	0.22
	dC_{11}/dP	10.67	10.66	10.62
EuP	dC_{12}/dP	1.94	1.93	1.92
	dC_{44}/dP	-0.04	-0.04	-0.03
	dC_{11}/dP	11.00	11.01	10.9
EuAs	dC_{12}/dP	1.89	1.88	1.87
	dC_{44}/dP	-0.08	-0.08	-0.08
	dC_{11}/dP	11.76	11.75	11.73
EuSb	dC_{12}/dP	1.80	1.79	1.77
	dC_{44}/dP	-0.18	-0.18	-0.18

Table 2 — B, G, Cs (in 10^{10} Nm^{-2}), σ, A and G/B for EuX (X= N, P, As and Sb) at 300K

Material	B	G	σZ_A		C_s	G/B
EuN	3.81	2.45	0.71	1.03	2.42	0.64
EuP	2.60	1.94	0.50	0.62	2.22	0.75
EuAs	2.39	1.83	0.46	0.57	2.14	0.77
EuSb	2.02	1.64	0.39	0.47	1.99	0.81

The bulk modulus notified the impact of the pressure on the elastic behaviour of a solid. The bulk modulus is interpreted as the proportion of the applied pressure as stress to the volume as longitudinal strain. On decreasing or increasing applied pressure the volume of a material decreases or increases, which regains to its original volume when the pressure is removed. The value of bulk modulus (B) for EuN is greater compare to EuP, EuAs, EuSb. This represents that EuN to be tougher and less soft than to EuP, EuAs, EuSb. The toughness to fractureratio[18] *i.e.*, (G/B) > 0.57 demonstrates the brittle behaviour of the europium monopnictides. The nature of interatomic forces is changing from non-central to central as the value of σ is greater than 0.5 for EuN which is prerequisite condition for non-central. The acoustical velocities of EuX are found out using Eqs. (12)-(16). The evaluated values of longitudinal, shear and Debye average velocities (V_L, V_S, V_D) along <100>, <110>, <111> directions with in temperature regime 100-300K are depicted in Table 3.

The acoustical velocity in shear mode (V_S) is highest along <110>polarized in<1$\bar{1}$0>for EuN and lowest for EuSb along <110> and polarized in<001>orientation. The longitudinal velocity (V_L) is maximum for EuP along <111> direction.

Table 3 indicates that the Debye mean velocity (V_D) is greatest along <100> for EuN & EuP and in<111> direction for EuAs and EuSb. So the direction <100> for EuN & EuP and <111> for EuAs and EuSb will be most preferred direction for acoustical wave transmission. The Debye average velocity of EuX is increasing with temperature in similar way as in the case of cerium monopnicties[17].

The estimated values of ultrasonic Grüneisen parameters at 300K are given in Table 4 along different directions for EuX. Grüneisen parameters give the thermophysical properties of the given materials like change in elastic constants with respect to temperature and thermal expansion of solids[19]. The average value of Grüneisen parameter are highest along <100> for EuX and lowest along <110>orientation. In case of average square Grüneisen parameters the longitudinal mode is greater than shear mode in<100> direction while shear mode dominates over longitudinal modes in <110> and <111> directions. The ultrasonic Grüneisen parameters are found to be highest for EuSb.

The Debye temperature refers to the crystal's maximum normal mode of oscillations. The Debye

Table 3 — V_L, V_S, V_D (in 10^3 m/s) of EuX (X= N, P, As and Sb) along <100>, <110>&<111> directions in the temperature range 100-300K

Materials	Direction	Velocity	100K	200K	300K
EuN	<100>	V_L	2.77	2.80	2.84
		$^*V_{S1=VS2}$	1.68	1.69	1.69
		V_D	2.15	2.15	2.17
	<110>	V_L	2.83	2.84	2.85
		$^\$V_{S1}$	1.68	1.69	1.69
		$^\#V_{S2}$	2.22	2.28	2.35
		V_D	2.06	2.06	2.09
	<111>	V_L	2.86	2.86	2.86
		$^@V_{S1}=V_{S2}$	1.61	1.64	1.67
		V_D	2.10	2.12	2.15
EuP	<100>	V_L	2.81	2.85	2.91
		$^*V_{S1}=V_{S2}$	1.44	1.44	1.45
		V_D	2.92	1.92	1.94
	<110>	V_L	2.64	2.66	2.68
		$^\$V_{S1}$	1.44	1.44	1.45
		$^\#V_{S2}$	2.44	2.51	2.60
		V_D	2.87	1.88	1.90
	<111>	V_L	3.58	2.59	2.60
		$^@V_{S1}=V_{S2}$	1.63	1.67	1.71
		V_D	2.06	2.09	2.13
EuAs	<100>	V_L	2.59	2.63	2.68
		$^*V_{S1}=V_{S2}$	1.29	1.28	1.29
		V_D	1.72	1.73	1.74
	<110>	V_L	2.40	2.41	2.43
		$^\$V_{S1}$	1.29	1.28	1.29
		$^\#V_{S2}$	2.27	2.34	2.42
		V_D	1.69	1.69	1.70
	<111>	V_L	2.34	2.34	2.34
		$^@V_{S1}=V_{S2}$	1.52	1.54	1.58
		V_D	1.88	1.91	1.94
EuSb	<100>	V_L	2.41	2.46	2.51
		$^@V_{S1}=V_{S2}$	1.12	1.12	1.13
		V_D	1.21	1.53	1.54
	<110>	V_L	2.18	2.19	2.21
		$^\$V_{S1}$	1.12	1.12	1.13
		$^\#V_{S2}$	2.16	2.24	2.31
		V_D	1.49	1.50	1.51
	<111>	V_L	2.10	2.10	2.10
		$^@V_{S1}=V_{S2}$	1.40	1.44	1.48
		V_D	1.73	1.76	1.79

Where *, $, # and @ indicate that the shear wave is polarized along <100>, <001>, <1$\bar{1}$0> and <$\bar{1}$10>orientations respectively.

temperature interlinks the elastic properties to thermophysical properties such as lattice enthalpy, thermal expansion, specific heat capacity and thermal conductivity[20]. The Debye temperature (θ_D) has been compute by utilizing the Eq. (17) and is presented in Fig. 3. From Figs. 3(a-d) it has been found that the values of θ_D are highest for EuN and lowest for EuSb along all chosen directions. Debye temperature for EuX is increasing in linear manner with temperature increase. Thus occupancy of phonon density is maximum for EuN and minimum for EuSb. The

Table 4 — Gruneisen parameters of EuX (X= N, P, As and Sb) in ⟨100⟩, ⟨110⟩ and ⟨111⟩ at 300K

Material	Direction	$\langle\gamma_i^j\rangle_L$	$\langle(\gamma_i^j)^2\rangle_L$	$\langle(\gamma_i^j)^2\rangle_{S1}$	$\langle(\gamma_i^j)^2\rangle_{S2}$
EuN	<100>	0.43	1.54	0.11	0.11
	<110>	-0.72	1.98	0.12	2.55
	<111>	-0.62	1.81	1.75	1.75
EuP	<100>	0.42	1.77	0.11	0.11
	<110>	-0.70	2.19	0.19	3.14
	<111>	-0.64	1.49	2.14	2.14
EuAs	<100>	0.41	1.83	0.11	0.11
	<110>	-0.69	2.27	0.09	3.29
	<111>	-0.64	1.93	2.24	2.24
EuSb	<100>	0.41	1.97	0.12	0.12
	<110>	-0.69	2.44	0.09	3.62
	<111>	-0.66	2.02	2.45	2.45

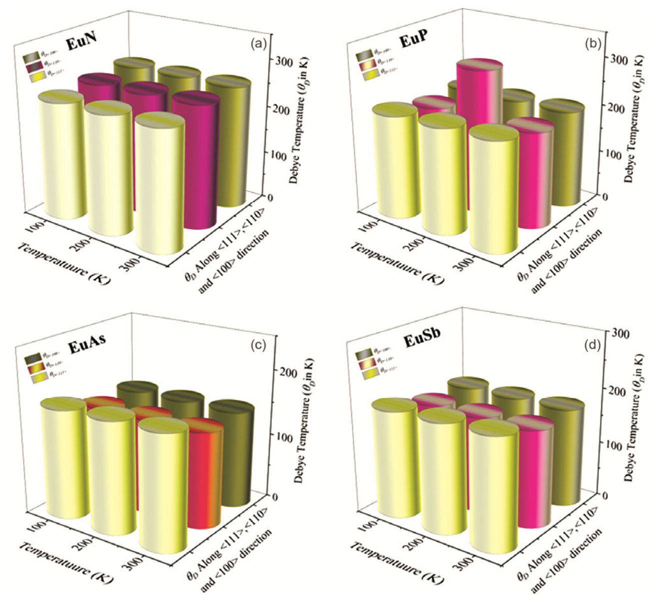

Fig. 3 — Debye temperature θ_D verses temperature for (a) EuN (b) EuP (c) EuAs(d) EuSb along <100>, <110>&<111> direction

Debye temperature is a very predominant quantity to define various thermophysical phenomenons. We are exploring Debye temperature for further studies to find thermal conductivities, specific heat, energy densities and thermal rela xation times like very interesting parameters.

4 Conclusions

We investigated the following point for europium monopnictides EuX (X= N, P, As and Sb) materials:

1 The computation of 2[nd]and 3[rd] order elastic constants (SOECs and TOECs) for europium monopnictides EuX (X= N, P, As and Sb) have been done successfully in the temperature span 100 to 300K successfully using the simple Born model.

2 The value of shear modulus and bulk modulus are higher for EuN material as compared to other europium monopnictides material, this indicates that the EuN is than the europium monopnictides.

3 The toughness fraction ratio *G/B*>0.59, it decides the chosen the europium monopnictides are brittle in nature.

4 The europium monopnictides satisfies the Born stability criterion. So the europium monopnictides are the mechanically stable.

5 The ultrasonic velocities in EuN are higher than that of other europiummonopnictides. So EuN is very usefulsubstance for ultrasonic wave transmission.

6 The Debye mean velocity rises with rise in the value of temperature as expected.

7 The ultrasonic Grüneisen parameters decrease with rise in the temperature as expected.

8 Longitudinal mode of Grüneisen parameter is dominant over shear mode along <100> direction.

9 The Debye temperature of EuX increases linearly with temperature along <100>, <110> and <111> direction.

The investigated results in present paper are very useful for their industrial applications and further researches.

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