



Original Article

Pressure-Induced Modulation of Electronic, Elastic, and Optical Traits in Hexagonal La_2O_3 for Advanced Solid-state Battery Cathode Frameworks

Vivek Chaurasiya, Pramod Kumar Yadawa*

*Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research,
V. B. S. Purvanchal University, 222003, Jaunpur, India*

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Abstract: In this study, we systematically investigate the composition-dependent elastic, mechanical, and thermophysical properties of the hexagonal close-packed (HCP) structured rare-earth metal chalcogenide, lanthanum oxide La_2O_3 , at a constant temperature of 300 K. Atomistic simulations were executed across a hydrostatic pressure range of 0–100 GPa using the well-established Lennard-Jones (L-J) interatomic potential model. This potential framework was utilized to compute the pressure-dependent limiting values of the Second-Order Elastic Constants (SOECs) and Third-Order Elastic Constants (TOECs). Leveraging these evaluated elastic coefficients, we determined the longitudinal and shear acoustic wave velocities, alongside the direction-dependent ultrasonic attenuation, for the constituent elements (La and O) within the La_2O_3 lattice matrix. Furthermore, key engineering metrics-including the bulk modulus, shear modulus, Young's modulus, and Poisson's ratio-were calculated to evaluate the high-pressure mechanical stability and deformation behavior of hexagonal La_2O_3 . Interestingly, the bulk modulus exhibits a consistent linear increase at ambient pressure corresponding to localized atomic variations. This monotonic enhancement correlates with minimized ultrasonic attenuation values, thereby confirming the heightened structural ductility and mechanical resilience of the compound under extreme environments.

Keywords: Rare-earth metal chalcogenide, Elastic constants, Ultrasonic velocity, Ultrasonic attenuation.

1. Introduction

The first element in the series, lanthanum (La), is the source of the nomenclature for the class of chemical elements known as lanthanides, or rare earth elements [1]. The solid material known as

* Corresponding author.

E-mail address: VivekChaurasiya25@gmail.com

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lanthanum oxide (La_2O_3) is white in colour, odourless, and soluble in weak acids but insoluble in water. The interaction between localized and itinerant states is essential in determining the physical and chemical properties of La_2O_3 , a fundamental f-electron system [2]. Lanthanum oxide's P-type semiconductor behavior explains why its resistance decreases with temperature.

Thermodynamic stability is demonstrated by lanthanum oxide (La_2O_3), which also has a large band gap [3] and a notable dielectric constant [3, 4]. As a result, this material has great potential for a number of uses in the industrial and technological spheres. White light emitting diodes, medical diagnostics, high definition televisions, camera lenses, telescopes, microscopes, cathode ray tubes, and fingerprint detection are just a few of the applications for lanthanum oxide [4]. According to a study by Xu et al., the compound La_2O_3 has been studied as a possible medium for phosphor materials intended for the incorporation of lanthanide ions [4, 5].

However, because La_2O_3 is sensitive to environmental factors, care must be taken when working with it. More specifically, it has a quick propensity to react chemically with atmospheric moisture, producing lanthanum hydroxide ($\text{La}(\text{OH})_3$). Furthermore, La_2O_3 can react with carbon dioxide in the presence of moisture to produce carbonates [5]. The production of electrodes, fluorescent lamps, optical fibers, and radiation-related applications are just a few of the uses for lanthanum fluoride. This material is highly prized in complex devices and contemporary technology due to its remarkable optical qualities and widely reported luminescence features [6].

The subject of undoped La_2O_3 has been thoroughly studied in the [5]. Nonetheless, publications that concentrate on La_2O_3 phosphors, like $\text{La}_2\text{O}_3:\text{Eu}$ [1, 7] and $\text{La}_2\text{O}_3:\text{Ho}$ [8], noticeably neglect the impact of this factor. As demonstrated by recent studies like those by Dey et al., the significance of La_2O_3 in phosphor studies has frequently been disregarded [9]. Nonetheless, it is imperative that this subject receive the attention it merits. Theoretical aspects of impurity doping in lanthanum oxide have been studied recently. Umezawa et al., found that coordination number affects silicon stability at substitutional sites [10]. Bannikov et al., conducted a study. investigated the electronic and magnetic properties of nitrogen-doped lanthanum sesquioxide (La_2O_3) using the ab-initio method [10] to improve the photoluminescence properties of La_2O_3 through impurity doping, numerous experimental studies using chemical synthesis and other techniques have been conducted [11]. Conducting first-principles investigations on rare earth oxides has become increasingly popular in recent years. This interest stems from their important role in both basic science and practical applications. It is commonly known that applying pressure causes a material's characteristics to change. Therefore, thorough research into the characteristics and qualities of materials used in high-pressure environments, like space missions and space shuttles, is essential.

The investigation of pressure-induced properties in the hexagonal phase of La_2O_3 has not yet been documented, as far as we are aware. This work provides a thorough examination of the optical and structural characteristics of hexagonal phase La_2O_3 under various pressure conditions. Numerous studies have shown that hexagonal La_2O_3 has a lot of promise as a material for pressure-dependent systems. A useful framework for investigating the optoelectronic properties of the hexagonal La_2O_3 will be provided by the current studies.

2. Computational Theory

2.1. Elastic Constants

To provide a concise description of the material's physical and mechanical properties as well as its anisotropic attenuation behavior, several theoretical approaches are available in addition to experimental methods that can be used to examine the previously mentioned characteristics through formulation. Among the researchers, the well-known Lennard-Jones interaction potential techniques are widely employed because of their high level of accuracy in producing results according to experimental

standards. This evaluation provides definitions for the additional-order elastic constants, including the experimental material referred to as second-order (SOEC) and its third order (TOEC) value, and this potential model's evaluation technique demonstrates how the second-order elastic constants connected to materials with a hexagonal structure are influenced by the lattice parameters [12].

$$C_{IJ} = \frac{\partial^2 U}{\partial e_I \partial e_J}; \quad I \text{ or } J = 1 \dots 6 \quad (1)$$

$$C_{IJK} = \frac{\partial^3 U}{\partial e_I \partial e_J \partial e_K}; \quad I \text{ or } J \text{ or } K = 1 \dots 6 \quad (2)$$

In addition, the general potential formulation for the Lennard-Jones model is well defined by

$$\varphi(r) = -\frac{a_0}{r^m} + \frac{b_0}{r^n}$$

Where, $a_0 = 4\varepsilon\sigma^m$, and $b_0 = 4\varepsilon\sigma^n$ here m and n are fitting parameters and ε and σ are the inter-atomic potential parameters.

Equations 4 and 5 represent general mathematical simplifications for SOECs and TOECs, where the third-order elastic constants (TOECs) are decomposed into ten fundamental parametric forms, and the second-order elastic constants (SOECs) into six [13]. This decomposition facilitates further simplification processes, enabling precise theoretical evaluation of the material properties previously described. These formulations for SOECs and TOECs are detailed in Equations 4 and 5 [13], respectively

$$\left. \begin{aligned} C_{11} &= 24.1 p^4 C' \\ C_{12} &= 5.918 p^4 C' \\ C_{13} &= 1.925 p^6 C' \\ C_{33} &= 3.464 p^8 C' \\ C_{44} &= 2.309 p^4 C' \\ C_{66} &= 9.851 p^4 C' \end{aligned} \right\} \quad (3)$$

Here, where $p = c/a$, is an axial ratio for the hexagonal material or compound and

$$C' = \chi a / p^5$$

$$B\psi a^3 = /p^3$$

$$\chi = (1/8)[\{n - m\} / \{a^{n+4}\}]$$

$$\psi = -\chi / \{6 a^2 (m + b_0 (nn + 6))\}$$

Is evaluated using integer values, and the Lennard-Jones potential variable, b_0 , [12] is widely known. Additionally, these characteristics may be changed even with a small change in temperature or attenuation [14] because they are incredibly dependent on these factors.

2.2. Ultrasonic Velocity, Related Parameters and its Theoretical Evaluation

Solids' mechanical characteristics differ from fluids in two significant ways. Shear stress is supported by the stronger binding forces between the atoms of these materials. Anisotropy can develop in single crystals when atoms form a regular lattice. Ultrasonic wave velocity may be calculated using elastic moduli (Y , G , and σ) and material density (d). Logitudinal and shear wave velocities (V_L and V_S) may be calculated using the following formulas. Ultrasonic velocities may be represented using lame's moduli (δ and μ) as follows:

$$V_L = \sqrt{\frac{\delta + 2\mu}{\rho}} \quad (4)$$

And

$$V_T = \sqrt{\frac{\mu}{\rho}} \quad (5)$$

The transverse and longitudinal sound velocities in a polycrystalline system are used to get the average sound velocity using the following formula [15]:

$$V_M = \left[\frac{1}{V_L^3} + \frac{1}{V_T^3} \right]^{-\frac{1}{3}} \quad (6)$$

The stress-strain relationships for anisotropic crystals change according to orientation. Thus, the velocity of an ultrasonic wave varies with the wave's propagation direction and polarization mode. There are three types of ultrasonic velocity (one longitudinal and two-shear wave) for each direction of wave propagation in hexagonal and hexagonal structured materials.

3. Thermophysical Parameters

3.1. Debye Temperature

The Debye temperature (Θ_D) refers to the temperature at which a material's phonon wavelength closely matches its interatomic spacing. It also draws a distinction between the classical and quantum properties of lattice vibrations. This temperature can be used to distinguish between a solid's high and low temperature behavior. The Debye temperature is critical for understanding numerous thermophysical properties of solids, such as melting temperature, bonding forces, thermal conductivity, the energy necessary for the formation of vacancies, specific heat, phonon dynamics, and superconductivity. When $T > \Theta_D$, all vibrational modes have almost equal energy ($k_B T$). However, for $T < \Theta_D$, higher frequency modes are locked. There are several ways for estimating the Debye temperature. When temperatures are low, only acoustic modes cause vibrational excitations. As a result, at low temperatures, the Debye temperature predicted from elastic constants is consistent with that determined from specific heat measurements. In this work, the Debye temperature of La_2O_3 is estimated using the Anderson approach, employing the following equation [16].

$$\Theta_D = \hbar V_D \frac{(6\pi^2 n_a)^{\frac{1}{3}}}{K_B} \quad (7)$$

where n is the number of atoms in a unit cell, V_0 is its volume, k_B is Boltzmann's constant, $\hbar$ is Planck's constant, and V_M is the mean sound velocity. The Debye temperature of hexagonal La_2O_3 in its ground state, which is around 380 K. (a) (b) La_2O_3 has a modest Debye temperature, indicating that the atomic bonding strengths are not very strong and that the material under examination is not very hard.

Here, $\hbar$ is the quantum of action, which is equal to Planck's constant divided by 2π . K_B is the Boltzmann Constant, and n_a is the atom concentration.

3.2. Debye Average Velocities

The Debye average velocity is a significant metric in low-temperature physics because it is connected to elastic constants via ultrasonic velocities. The Debye average velocity (V_D) in materials is derived using the following equation

$$V_D = \left[\frac{1}{3} \sum_{i=1}^3 \int \frac{1}{V^3} \frac{d\Phi}{4\pi} \right]^{-1/3} \quad (8)$$

And along the [110] (for cubic) and any angle with the unique axis of hexagonal structured crystal, direction of propagation, the equation (4) reduces as:

$$V_D = \left[\frac{1}{3} \left(\frac{1}{V_L^3} + \frac{1}{V_{s1}^3} + \frac{1}{V_{s2}^3} \right) \right]^{-1/3} \quad (9)$$

The theoretical assessment of ultrasonic velocity and Debye average velocity in hexagonal materials may be done using formulas written in the [100] direction, assuming knowledge of elastic constants.

$$\begin{aligned} [100] V_L &= \sqrt{\frac{C_{11}}{2\rho}} \\ [001] V_{S1} &= \sqrt{\frac{C_{44}}{\rho}}, \quad [010] V_{S2} = \sqrt{\frac{(C_{11}-C_{12})}{2\rho}} \end{aligned} \quad (10)$$

[001] direction:

$$\begin{aligned} [001] V_L &= \sqrt{\frac{C_{33}}{\rho}} \\ [100] V_{S1} &= [010] V_{S2} = \sqrt{\frac{C_{44}}{\rho}} \end{aligned} \quad (11)$$

Moreover, an angular dependency of these above mentioned velocities are depicted here

$$\left. \begin{aligned} V_L^2 &= \{C_{33} \cos^2 \theta + C_{11} \sin^2 \theta + C_{44} \\ &\quad + \{[C_{11} \sin^2 \theta - C_{33} \cos^2 \theta \\ &\quad + C_{44} (\cos^2 \theta - \sin^2 \theta)]^2 \\ &\quad + 4 \cos^2 \theta \sin^2 \theta (C_{13} + C_{44})^2\}^{1/2}\} / 2\rho \\ V_{S1}^2 &= \{C_{33} \cos^2 \theta + C_{11} \sin^2 \theta \\ &\quad + C_{44} - \{[C_{11} \sin^2 \theta - C_{33} \cos^2 \theta \\ &\quad + C_{44} (\cos^2 \theta - \sin^2 \theta)]^2 \\ &\quad + 4 \cos^2 \theta \sin^2 \theta (C_{13} + C_{44})^2\}^{1/2}\} / 2\rho \\ V_{S2}^2 &= \{C_{44} \cos^2 \theta + C_{66} \sin^2 \theta\} / \rho \end{aligned} \right\} \quad (12)$$

Where V_L represents longitudinal sound velocity, ρ represents crystal density, and V_{S1} and V_{S2} are the first and second transverse acoustic modes, respectively. Below Table shows the calculated sound velocities for various directions. The longitudinal velocity of La_2O_3 along [100] is much greater than that along [001].

Also to evaluate the density the formula can be used to determine it for material with a hexagonal structure [14, 18, 19].

$$d = \frac{2Mn}{3\sqrt{3}a^2cN_A} \quad (13)$$

Table 1. Anisotropic sound velocities (in 10^3 m/s) in La_2O_3 along principal crystallographic directions

Direction of propagation	Direction of polarization	Type of wave	Velocity (in 10^3 m/s)
001	001	Long.	4.594
	Any direction in 001 plane V_{S1}	Shear	5.512
	001 V_{S2}	909.03	5.512
100 (or any other direction perpendicular to 001)	100	Long.	3.602
	001 V_{S1}	Shear	9.878
	010 V_{S2}	Shear	2.717
At angle θ with the unique axis of the crystal		Long.	1.538
		Shear	7.424
		Shear	7.424

Due to the advanced engineering application of experimental HCP material in a temperature and composition limit, it becomes important to investigate their thermophysical behavior at those extreme

conditions. Utilizing the Debye model of heat capacity, we have calculated the thermal energy densities (E_0) and heat capacity (C_V) [20].

Within the scope of these experiments, the period taken during thermodynamic phonons to reassemble themselves following the propagation of an ultrasonic wave is known to be the corresponding thermal relaxation time (τ). It has a direct relationship with specific heat (C_V), Debye average velocity, and thermal conductivity (k) [20].

$$\tau = \tau_S = \tau_L/2 = \frac{3k}{C_V V_D^2} \quad (14)$$

3.3. Mechanical Property

Based on the experimental analysis of the evaluated physical properties, the material's stability, crystal structure, thermal conductivity, mechanical strength, and hardness can be reliably inferred from the calculated second-order elastic constants (SOECs). Furthermore, the Voigt–Reuss–Hill (VRH) approximation[21] has been employed to investigate variations in key mechanical parameters, including Pugh's ratio (B/G), Young's modulus (Y), Poisson's ratio (σ), bulk modulus (B), and shear modulus (G) [21, 22]. The standard relationships for these parameters within the VRH framework are expressed below in Equation [22]:

$$\begin{aligned} B_R &= \frac{C^2}{M} \\ M &= C_{11} + C_{12} + 2C_{33} - 4C_{13} \\ C^2 &= (C_{11} + C_{12})C_{33} - 4C_{13} + C_{13}^2 \\ B_V &= \frac{2(C_{11} + C_{12}) + 4C_{13} + C_{33}}{9} \\ B &= \frac{B_V + B_R}{2}, \quad G = \frac{G_V + G_R}{2} \quad (15) \\ G_V &= \frac{M + 12(C_{44} + C_{66})}{30} \\ G_R &= \frac{5C^2 C_{44} C_{66}}{2[3B_V C_{44} C_{66} + C^2(C_{44} + C_{66})]} \\ Y &= \frac{9GB}{G+3B}, \quad \sigma = \frac{3B-2G}{2(3B+G)} \quad (16) \end{aligned}$$

The lattice thermal conductivity (κ) was evaluated by following the Morelli and Slack [43] approach, which is given as equation 14:

$$k = AMT_D^3 \delta^3 / \gamma^2 T n^{2/3} \quad (17)$$

M (in amu) is the average atomic mass, θ_D is the Debye temperature, T is the temperature, δ is the amount of volume for each atom, γ is the Grüneisen number, and A represents the proportional constant. n is the total number of atoms per unit cell. Here the Grüneisen number determines the numerical value for the constant 'A', which is stated as follows.

$$A = 2.43 \times 10^{-8} / \left(1 - \frac{0.514}{\gamma} + \frac{0.228}{\gamma^2}\right)$$

γ is the Grüneisen number [23], which can be determined by $\gamma = \alpha B / (C_V \rho)$ [23], where α is the thermal volume expansion coefficient, B is bulk modulus, C_V is the heat capacity, and ρ is density of the material.

The relative values of the melting temperatures (T_m) of hexagonal crystals [24] is also dependent on the value of certain elastic constants C_{11} and C_{33} which are defined as [20, 25, 26], melting temperatures (T_m)

$$T_m = 354 + \frac{4.5(2C_{11} + C_{33})}{3} \quad (18)$$

where C_{11} and C_{33} are in GPa [27], and T_m is in K.

4. Attenuation

Here, we could observe that in a viscous medium by the transfer of momenta carries the energy of the electrons in the normal state, is been carried and from the lattice vibrations via a novel way. The mechanism is also known as the electron-viscosity mechanism. The ultrasonic attenuation produced by energy loss owing to shear and compressional viscosities of electron gas for longitudinal (α) Long and shear waves (α) Shear is given as [28]:

$$\alpha_{long} = \frac{\omega^2 f^2}{2\rho V_l^3} \left(\frac{4}{3} \eta_e + \chi \right) \quad (19)$$

$$\alpha_{shear} = \frac{\omega^2}{2\rho V_s^3} \eta_e \quad (20)$$

where η_e and χ represent the electronic shear and compressional viscosities of electron gas.

4.1. Attenuation Due to Phonon–Phonon Interaction

The energy quanta associated with mechanical waves are known as phonons. Ultrasound waves (acoustic phonons) alter the state of equilibrium distribution of the thermal phonons in solids. The relaxation process ensures that thermal phonons return to equilibrium. The process generates entropy, which results in absorption. The notion of modulated thermal phonons offers the following formula for calculating the absorption coefficient of an ultrasonic wave caused by phonon-phonon interaction in materials. (α)_{akh} [28-30]:

$$\alpha_{akh} = \alpha_{pp} = \frac{\omega^2 \tau \delta C}{2\rho(1+\omega^2 \tau^2) V^3} \quad (21)$$

Where τ is the thermal relaxation time (the time required for the re-establishment of the thermal phonons) and V is longitudinal or shear wave velocity. C_Δ is change in elastic moduli caused by stress (by passage of ultrasonic wave) and is given as:

$$\delta C = 3E_0 < \gamma_i^j >^2 - < \gamma_i^j >^2 C_V T$$

Here E_0 is the thermal energy density. ΔC is related with the acoustic coupling constant (D), which is the measure of acoustic energy converted to thermal energy due to relaxation process and is given by the following expression [29]:

$$D = \frac{3\delta C}{E_0} = 9 < \gamma_i^j >^2 - 3 < \gamma_i^j >^2 \frac{C_V T}{E_0}$$

Using equation (16c), the equation (16a) takes the following form under condition $\omega \tau < 1$

$$\alpha_{akh} = \alpha_{pp} = \frac{\omega^2 \tau E_0 D}{6\rho V^3} \quad (22)$$

4.2. Attenuation Due to Magnon-phonon Interaction

Ferromagnetic along with ferroelectric materials are made up of 'domains', which are elementary areas with distinct magnetic or electric polarizations. These domains are aligned in a variety of orientations, but are often orientated along the polarization vector known as the direction of easy magnetization (or electrification). These are typically orientated along the primary crystallographic axis. A ferromagnetic material's hexagonal crystal contains six simple magnetization orientations, which are arranged in either negative or positively orientated pairs along three perpendicular coordinate axes. Thus, two adjacent subdomains are synchronized at 900 or 1800. The total length of domains along the direction of polarization increases (or decreases) due to the Magnetostriction effect, given that the resulting magneto strictive strain provided is either positive or negative.

This causes an enhancement or decrease in elastic constants, depending on the corresponding sign of the magnetostrictive parameter. The overall magnitude of change is determined by the amount of stress applied. The phenomenon is known as the ΔE effect. When a ferromagnetic or as ferroelectric material is subjected to cyclic stress, such as an ultrasonic wave, the domain wall is shifted due to the ΔE effect, which leads to the hysteresis loop. Thus, ultrasonic energy is dissipated. The loss of each half cycle in unit volume is determined by the area of the hysteresis loop.

The ultrasonic attenuations in single crystal solids at high temperatures are mostly due to phonon-phonon interactions (Akhiezer loss) [19] and thermoelastic relaxation mechanisms (thermoelastic loss). The formulation for estimating ultrasonic attenuation due to phonon-phonon interactions was developed by [31] and is given by:

$$(\alpha/f^2)_{Akh} = 4\pi^2 \tau E_0 (D/3) / 2\rho V^3 \quad (22a)$$

The ultrasonic wave frequency is denoted by f , and the thermal energy density is denoted by E_0 . [32]

The thermoelastic loss $(\alpha/f^2)_{Th}$: [14] equation as follows

$$(\alpha/f^2)_{Th} = 4\pi^2 < \gamma_i^j >^2 \frac{kT}{2\rho V_L^5}$$

$$\alpha_{long} = \frac{2\pi^2 f^2}{\rho V_L^3} \left(\frac{4}{3} \eta_e + \chi \right) \quad (23)$$

$$\alpha_{shear} = \frac{2\pi^2 f^2}{\rho V_S^3} \eta_e \quad (24)$$

The total consequence of ultrasonic attenuation $(\alpha/f^2)_{Total}$, caused by the thermoelastic loss and Akhiezer losses exhibited in the longitudinal, shear mode of propagation, can be calculated as [35]:

$$(\alpha/f^2)_{Total} = (\alpha/f^2)_{Th} + (\alpha/f^2)_L + (\alpha/f^2)_S \quad (25)$$

Where $(\alpha/f^2)_{Th}$ is the thermoelastic loss, while $(\alpha/f^2)_L$ and $(\alpha/f^2)_S$ are the ultrasonic attenuation coefficients for the longitudinal wave and shear wave, correspondingly.

5. Elastic Anisotropy

While studying the crystalline-structured compound. Elastic anisotropy is a fundamental element that influences substance stability, both mechanically as well as structurally, under various directed loads. The term "anisotropy indices" refers to the corresponding directional mechanical characteristics of the planned system. Furthermore, elastic anisotropy allows us to control a wide range of physical processes, such as the growth concerning plastic type deformation inside a crystal, the propagation regarding micro-racks within solids, the alignment and misalignment of quantum dots, conductivity, also known to be phononic conductivity, and defect mobility. It can also predict the mechanical toughness from materials. Thus, understanding anisotropic behavior in material along with mechanical behavior is essential. Furthermore, anisotropy and isotropy are frequently prominent in crystals because of metallic & covalent (directional) bonding, respectively.

As a result, shear anisotropy factors are utilized to properly predict material behavior and quantify the degree of anisotropy in atomic bonds in crystal planes. In the case of hexagonal crystal symmetry, the three parameters given below can be utilized to estimate the crystal's shear anisotropy.

$$\begin{aligned} A_1 &= \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}} \\ A_2 &= \frac{4C_{55}}{C_{22} + C_{33} - 2C_{23}} \\ A_3 &= \frac{4C_{66}}{C_{11} + C_{22} - 2C_{12}} \end{aligned} \quad (25)$$

A_1, A_2, A_3 respectively illustrate the usual formulations for anisotropy as shear anisotropy coefficient for $\langle 100 \rangle, \langle 010 \rangle, \langle 001 \rangle$ surfaces across the $\langle 011 \rangle$ along with the $\langle 010 \rangle$ directions, $\langle 101 \rangle$ along with $\langle 010 \rangle$ directions, and in the direction of $\langle 110 \rangle$ along with $\langle 010 \rangle$. Because, in the scenario of hexagonal symmetry, with $C_{11} = C_{22}, C_{44} = C_{55}$, and $C_{13} = C_{23}$, thus our complete estimated values of A's are $A_1 = A_2$ and $A_2 = A_3$. If this criterion is fulfilled, we may infer that our crystalline substance is isotropic in terms of shear; if not, it is anisotropic. Below Table 2 presents the calculated values for shear anisotropy for La_2O_3 .

Furthermore, using the standard equations shown below, one can determine other types of anisotropy within the crystal symmetry, such as the universal anisotropy index (A^U), Zener anisotropy (A^{eq}), shear anisotropy (A^G), and compressibility anisotropy (A^B) for crystalline symmetric structure.

$$A^U = \frac{5G_V}{G_R} + \frac{B_V}{B_R} - 6 \geq 0, A^{eq} = \left(1 + \frac{5}{12}\right) + \sqrt{\left(1 + \frac{5}{12}A^U\right)^2} \quad (26)$$

$$A^G = \frac{G_V - G_R}{2B}, A^B = \frac{B_V - B_R}{2B}$$

This universal anisotropy index (A^U) is commonly used to measure the anisotropy of any crystalline material. Regardless of crystal symmetry, there is only one measure of anisotropy. Unlike other known anisotropy metrics, A^U considers both shear in addition to bulk contributions. We can conclude from Eq. (14).

G_V/G_R has a higher influence with respect to the anisotropy index (A^U) compared to G_V/G_R . A number less than or greater than zero shows varying degrees regarding anisotropy, whereas zero denotes an isotropic material. The calculated value of A^U for La_2O_3 is 2.10, indicating strongly anisotropic properties. For locally isotropic crystalline structures, $A^{eq} = 1.0$. At ambient pressure, La_2O_3 has an estimated A^{eq} value of .39, indicating its significant anisotropy. A^G and A^B have values ranging from zero to one. $A^G = A^B = 0$ represents optimum elastic isotropy, while $A^G = A^B = 1$ represents maximal elastic anisotropy.

6. Results and Discussion

6.1. Second Order and Third-Order Elastic Constant Evaluation for Hcp Transition Complex Composite Material La_2O_3

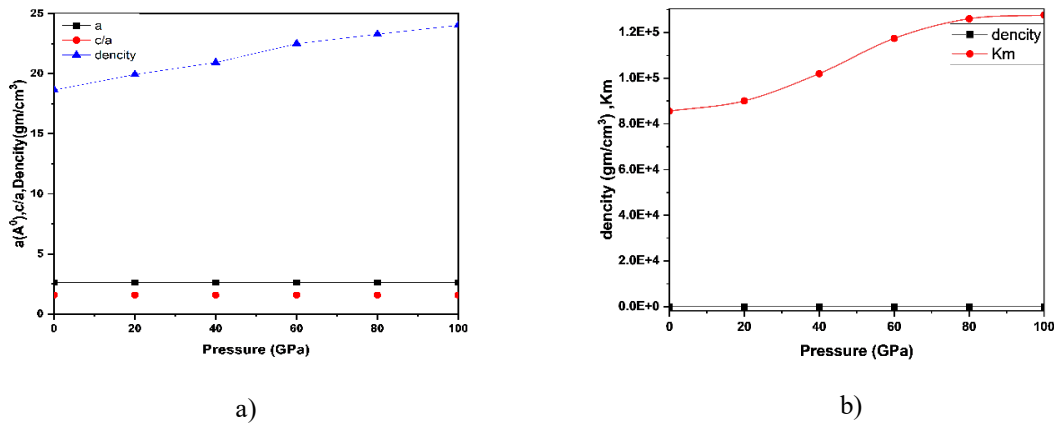


Figure 1. (a) The dedicated value of Lattice constant a (Å), Bessel plane distance c/a (b) relative density, and Thermal Relaxation constant K_m Vs HCP Transition material La_2O_3 .

In the present study HCP Transiton complex composit material La_2O_3 , we have successfully derived accurate values for various elastic coefficients-specifically six second-order elastic constants (SOECs) and ten third-order elastic constants (TOECs), using an interaction potential approach. Based on our theoretical framework and comparative analysis, the obtained results show strong agreement with available experimental data, exhibiting minimal deviations and confirming the validity of our model [18]. Additionally, we have determined the essential lattice parameters for HCP Transiton complex composit material La_2O_3 where “a” represents the basal plane lattice constant and “p” denotes the axial ratio ($p=c/a$) [33] for the hexagonal close-packed (HCP) structure [36]. The composition-dependent lattice constants a for comparative hexagonal rare-earth metals are as followed a 3.652 Å and c 5.586 Å as illustrated in Fig. 1(a). Corresponding densities of states (DOS) for each composition are also provided. The constant value of Leonard Jones potential constant “b0” is also evaluated with mathematical simulation manipulation technique and finally taken at 4.69×10^{-64} , 4.46×10^{-64} , 4.42×10^{-64} , 3.95×10^{-64} , 3.87×10^{-64} , 3.73×10^{-64} respectively for pressure values used.

Additionally, on the basis of the above-mentioned and evaluated data, the evaluated values of the second and third-order elastic constants Pressure of HCP Transiton complex composit material La_2O_3 is depicted in Fig. 2(a) and Fig. 2(b), respectively.

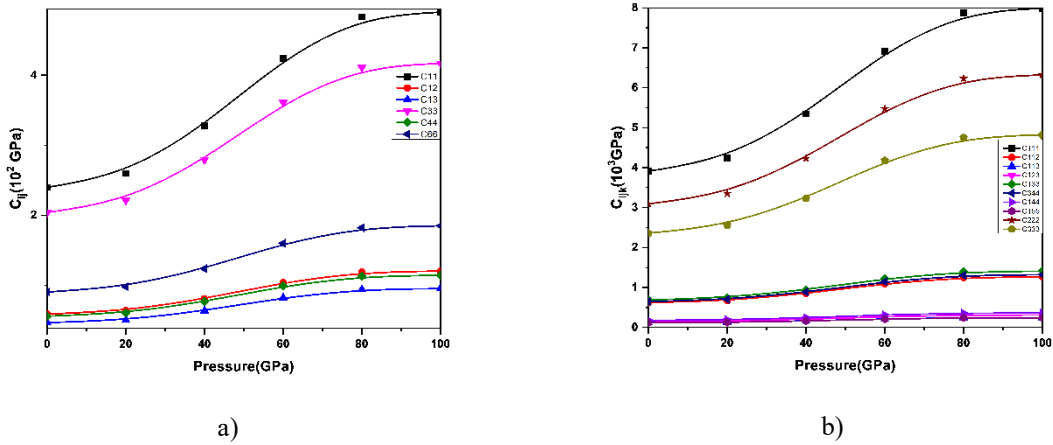


Figure 2. The variation in the respective values of (a) SOECs and (b) TOECs Vs HCP Transiton complex composit material La_2O_3

The above Fig. 2(a) depicts the evaluated variation of SOEC of HCP Transiton complex composit material La_2O_3 . On the basis of data analysis for the particular HCP complex material compound La_2O_3 , we can conclude that the negative values of TOECs indicate the presence of strain for the various pressure range for HCP Transiton complex composit material La_2O_3 . This is aligned with previous investigations on materials with hexagonal structures, affirming the theoretical framework's accuracy in valuing higher-order elastic coefficients. As a result, the theory used to investigate higher-order elastic coefficients is justified using Eqs. 1 and 2. For HCP structure material stability, here the five different SOECs (C_{ij} , namely C_{11} , C_{12} , C_{13} , C_{33} , and C_{44}) satisfy Born-Huang's norms[24]. This HCP Transiton complex composit material La_2O_3 is mechanically stable because it is evident that the positive elastic constant values satisfy Born-mechanical Huang's stability constraints defined as.

$$\begin{aligned} \dot{C}_{44} > 0, \dot{C}_{11} - |\dot{C}_{12}| > 0 \\ (\dot{C}_{11} + \dot{C}_{12}) \dot{C}_{33} - 2 \dot{C}_{213} > 0 \\ \text{Where } \dot{C}_{jj} = \dot{C}_{jj} - P, (P=1, 3, 5). \\ \dot{C}_{12} = C_{12} + P, \dot{C}_{13} = C_{13} + P \end{aligned}$$

6.2. Mechanical Property

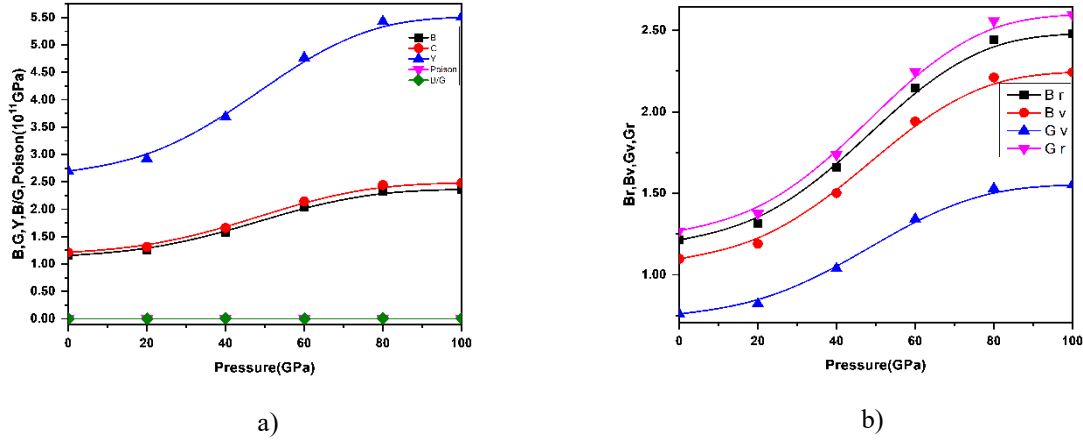


Figure 3. (a) B, G, Y, B/G, σ Vs (b) Br, Bv, Gv, Gr HCP Transition composited La_2O_3 .

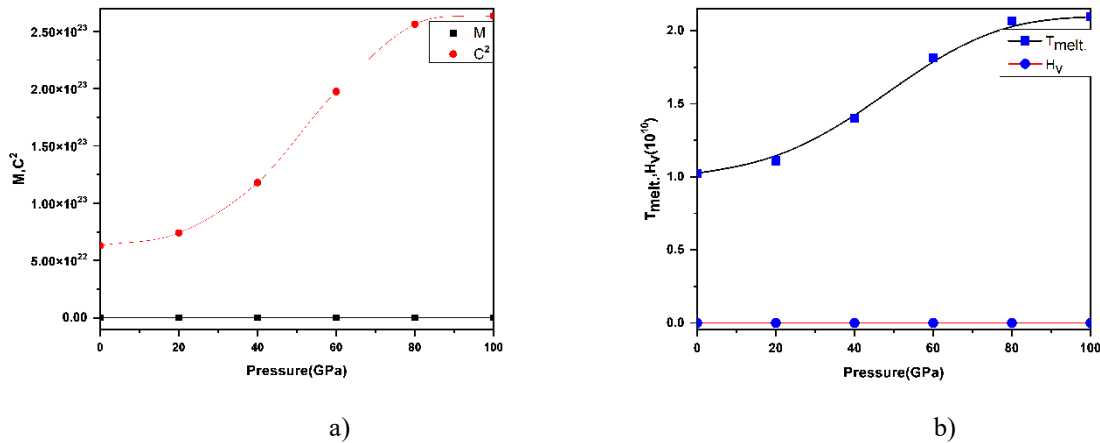


Figure 4. (a) M, C^2 , (b) melting temperature T_{melt} , Hardness H_v Vs HCP Transition complex composited material La_2O_3 .

The corresponding atomic volume of Transition Type Metal Compound La_2O_3 range volume decreases, as illustrated in Fig. 4(a). The values of bulk modulus (B), Young's modulus (Y), and shear modulus (G) for Transition Type Metal Compound La_2O_3 are observed to increase progressively with changes in composition. This trend reflects an enhancement in the stiffness and bonding strength of the nanomaterials. Additionally, the standard G/B ratio, which is >0.35 at STP, signifies a predominant ionic bonding character, and according our result we can conclude that our ratio within the range and hence La_2O_3 can be considered as ionic. This ratio, along with the B/G and Poisson's ratio (σ), provides valuable insights into the mechanical behavior of the materials, particularly in predicting their brittleness or ductility. Materials with $\sigma = 0.1 \leq 0.28$ are considered as brittle while materials with $\sigma = 0.28 \leq 0.50$ are considered as Ductile, and regarding our evaluated result we can conclude our material is Brittle with values of 0.111 and further if the $B/G > 1.75$ it can be concluded as Ductile and < 1.75 is concluded

as Brittle, and our material La_2O_3 is typically considered brittle with range of 0.952 [38]. Our results for B/G indicate that the Transition Type Metal La_2O_3 are brittle in nature with nanomaterial composition because they are under their critical levels. The value of σ , which should perfectly be less than 0.5 for elastic and stable materials, is found to be within an acceptable range for composite. B/G ratio below 0.175×10^{-1} typically signifies brittleness, which is consistent with the behavior observed in Compared Metals. In the below section, we have demonstrated the relative values of Voigt–Reus’ constants (M and C^2), B_r ($\times 10^{10} \text{ Nm}^{-2}$), B_v ($\times 10^{10} \text{ Nm}^{-2}$), G_r ($\times 10^{10} \text{ Nm}^{-2}$), G_v ($\times 10^{10} \text{ Nm}^{-2}$), Y ($\times 10^{10} \text{ Nm}^{-2}$) for above evaluated HCP metals are depicted in below Fig. 3(a) and (b).

In addition to the mechanical properties discussed above, the melting temperature serves as a critical parameter in the development of materials with enhanced thermal stability, ductility, and brittleness. The melting temperature (T_m) and hardness (H_v) of HCP Transition complex composite material La_2O_3 have been systematically investigated and are presented in Fig. 4(b), illustrating their variation as a function of composition.

Table 2. Various anisotropy constants with their relative poisson’s ratio for nanomaterial composition HCP complex compound La_2O_3 are

P	A^U	f^E	A_1	A_2	A_3	A^{eq}
0	-2.1066	0.86535	0.61798	34671285	1.21217E+11	0.3956834
20	-2.1066	0.86529	0.61797	37562230	1.31323E+11	0.3956834
40	-2.1066	0.86531	0.61797	47419365	1.65785E+11	0.3956834
60	-2.1068	0.86569	0.61811	61336929	2.14454E+11	0.3956834
80	-2.1066	0.86531	0.61797	69854807	2.44223E+11	0.3956834
100	-2.1067	0.86541	0.61801	70868560	2.4777E+11	0.3956834

Table 2 shows that under different pressure of HCP Transition complex composite material La_2O_3 are, AB has a higher percentage of anisotropy than AG. This suggests that the bulk modulus is less oriented than the shear modulus. A_1 , A_2 , and A_3 findings with nanomaterial are also displayed in Table 1. If $A^U = f^E = A^Z = 1$, the substance is an isotropic crystal. According to the findings, composition HCP complex compound La_2O_3 are an anisotropic crystal absent in any other circumstances. With nanomaterial, the universal anisotropic index (A^U) deviates from zero, which is known as the highly single crystal anisotropy [12].

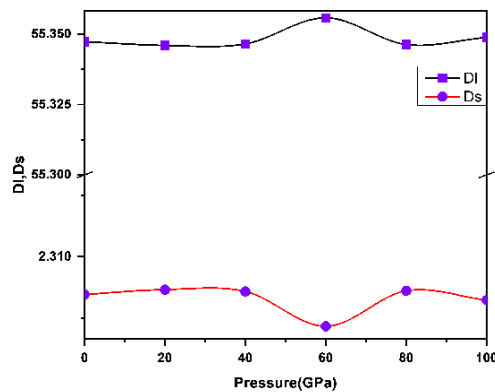


Figure 5. Variation of DL, DS Vs HCP Transition complex composite material La_2O_3 .

It is clear from Fig. 5 ure 8 that for all temperature, the values of D_S are larger than those of DL for all composition nanomaterials. It indicates that for the shear ultrasonic wave the transformation of ultrasonic energy into thermal energy is less than for the longitudinal ultrasonic wave.

6.3. Ultrasonic Velocity and Allied Parameters

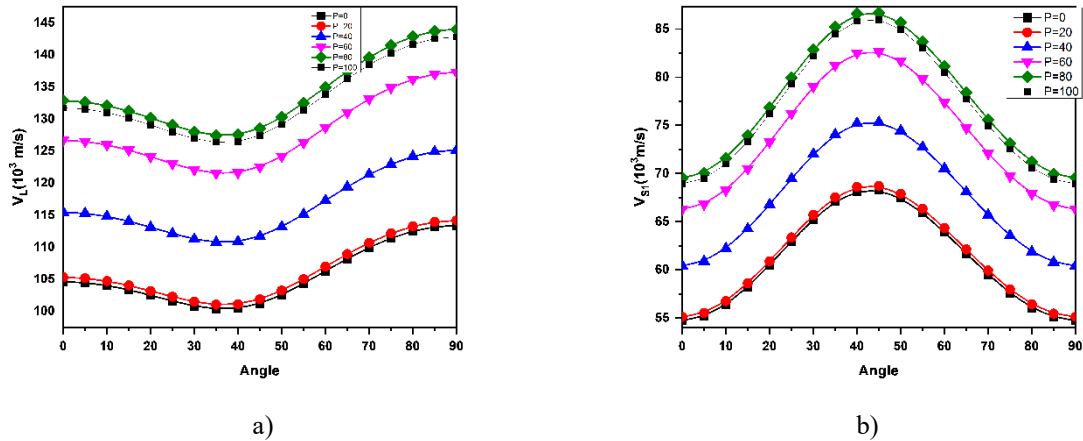


Figure 6. (a) Longitudinal velocity V_L (b) Shear velocity in Transverse direction V_{s1} vs. Attenuation Angle " Θ " for HCP Transition complex composite material La_2O_3

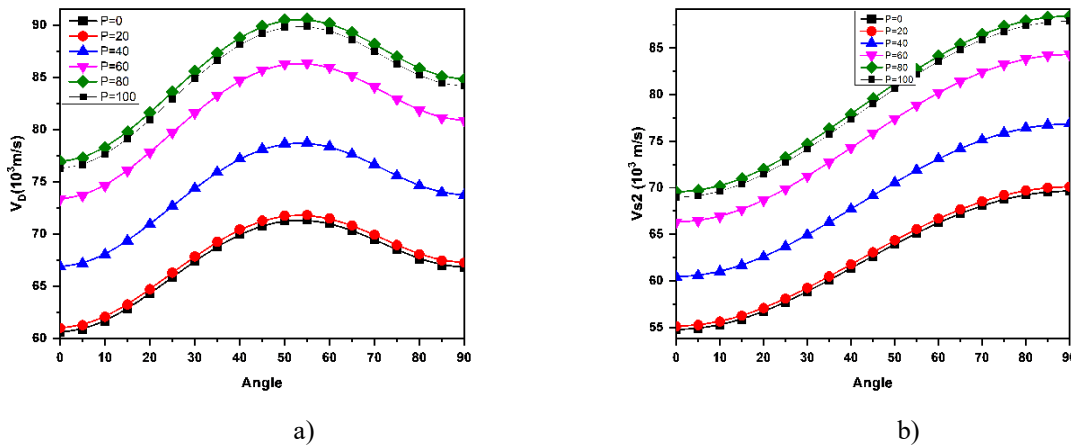


Figure 7. (a) Debey average velocity V_D , (b) Shear velocity V_{s2} vs Attenuation Angle " Θ " for HCP Transition complex composite material La_2O_3 .

The below Fig. 6, 7 demonstrate the angular dependency of ultrasonic velocities (V_L , V_{s1} , V_{s2} , V_D and T_0) with varying composition along the z-direction for the HCP Transition complex composite material La_2O_3 are in Fig. 6(a) and 6(b), the z-axis of the HCP Transition complex composite material La_2O_3 are correlates directly to the minima and maxima of the ultrasonic velocities V_L and V_{s1} . in addition, the value of V_{s2} is demonstrated in Fig. 6(b), and it is clear from the see-through that its values changes with the angular spread along the z-direction. The combined effects of SOECs and ρ (density) are held responsible in Favor of the uncharacteristic behavior of angle-dependent velocity. This effort's

discovery of the angle (Θ)-dependent velocity (V) curves is similar to those found for other hcp nanomaterials. This justifies the angle dependence of metal velocities [34]. Here, the V_D value decreased with increasing angle and reaches its minimum at 55.5° decreases from 5° from maxima value in Fig. 7(a). The relative value of the Debye average velocity is also influenced by the variation in the fundamental ultrasonic velocities, V_L , V_{S1} , and V_{S2} , which are used to evaluate V_D . Additionally, here When the z-axis of this crystal is at 45° , the average shear wave velocity shows a maximum.

In this section, Fig. 7 (b) presents a graphical depiction of the calculated thermal relaxation time, illustrating its variation with composition across different angular orientations. Here, the reciprocal characteristics of V_D , which are relative to $\tau \propto 3k/C_V V_D^2$ [24] is evaluated, and here we can conclude that the value of thermal relaxation time for the HCP Transiton complex composit material La_2O_3 is highly dependent on the value of the Fermi radius and can be affected by 'k'. The hexagonal structure of the HCP Transiton complex composit material La_2O_3 areis explained by the computation. The minimum value of the thermal relaxation time (τ) occurs along the wave propagation direction at an angle of 5° , indicating the shortest re-establishment time for thermally generated phonons and their equilibrium distribution. Consequently, the presence of phonon–phonon (p–p) interactions and the associated thermal relaxation give rise to ultrasonic attenuation observed in the material along this direction.

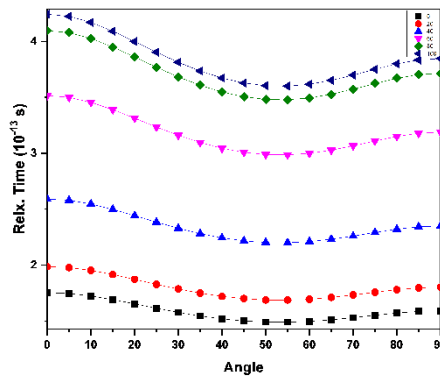


Figure 8. Relaxation time vs Attenuation Angle " Θ " with z- axis of crystal for HCP Transiton complex composit material La_2O_3 .

6.4. Ultrasonic Attenuation Due to Phonon-phonon Interaction and Thermal Relaxation Phenomena

In analyzing the ultrasonic attenuation, it is assumed that the wave flows along the z-axis of nanomaterial composition compound La_2O_3 . The Attenuation coefficient is alienated over frequency squared for longitudinal wave $(\alpha/f^2)_L$ and for shear wave $(\alpha/f^2)_S$ under the condition $\omega\tau \ll 1$ at various compositions is calculated using Eq. 11. The thermo-elastic loss by frequency squared (α/f^2) th is calculated using Eq. 25, and Fig. 8 illustrates the ultrasonic attenuation value resulting from the thermoelastic relaxation mechanism (α/f^2) .

It is assumed that the wave propagates down the z-axis of the HCP La_2O_3 compound when computing ultrasonic attenuation (UA). Eq. 23,24,25 is used for calculating the attenuation coefficient divided by frequency squared (α/f^2) Akh for the wave's longitudinal direction $(\alpha/f^2)_L$ and for the shear wave $(\alpha/f^2)_S$. Table 2 presented values of the composition-dependent longitudinal, shear and total attenuation of the compound La_2O_3 . Energy losses $(\alpha/f^2)_{Akh}$ are substantially proportional to D , E_0 , and V^3 . Thus, in the nanomaterial composition HCP Transiton complex composit material La_2O_3 are, E_0 and K have a significant impact on Akhieser losses. The thermo-elastic loss for the nanomaterial

composition HCP complex compound La_2O_3 is to be substantially less than the Akhieser loss, indicating that the p-p interaction mechanism-induced ultrasonic attenuation dominates over thermoplastic loss.

Total attenuation is mainly driven by two variables, namely thermal energy density and thermal conductivity. Thus, although nano material compositions of HCP Transition complex composite material La_2O_3 are the least ductile, they show their purest form at for different nanomaterial compositions and show additional ductility, as shown by the minimal attenuation. Hence, the nanomaterial composition HCP complex compound La_2O_3 are will have the lowest impurity content at ambient compositions.

In the present study, it is observed that ultrasonic waves predominantly propagate along the z-axis of the HCP Transition complex composite material La_2O_3 . Equations.22 and 22b clearly show that the Akh. Types of energy losses (α/f^2) Akh proportionate to D , E_0 , τ , and V^3 . are rising as atomic number (Z) increase in periodic table, as seen in Fig. 9. Therefore, in HCP Transition complex composite material La_2O_3 are, Consequently, the Akhieser losses in HCP transition metals are strongly influenced by the values of Energy and Corresponding temperature and the thermal conductivity K . A reduction in thermal conductivity leads to a notable increase in ultrasonic attenuation (UA). This suggests that UA is significantly governed by phonon–phonon (p–p) interaction mechanisms. However, due to the lack of sufficient experimental and theoretical data on ultrasonic attenuation in these specific materials, direct comparison and validation remain limited.

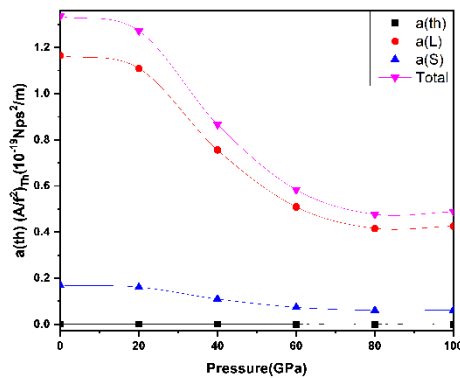


Figure 9. Attenuation Vs HCP Transition complex composite material La_2O_3

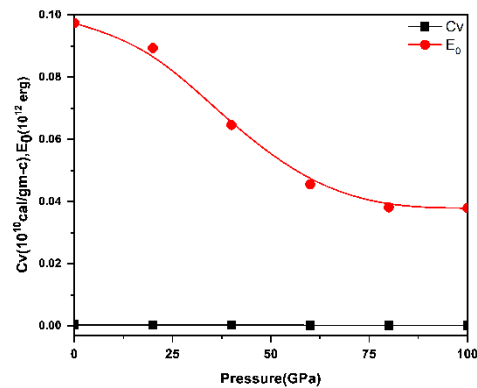


Figure 10. Energy and Specific Heat Vs HCP Transition complex composite material La_2O_3

As depicted in above graph the thermo-elastic loss in the nanomaterial composition HCP Transition complex composite material La_2O_3 arises significantly lower than the Akhieser loss. According to Equation (18), the primary contributor to total ultrasonic attenuation is Akhieser-type attenuation (UA), which is predominantly governed by phonon–phonon (p–p) interactions for both longitudinal and shear waves. The two key factors influencing total attenuation are thermal energy density and thermal conductivity.

The observed minimum attenuation values suggest that, although HCP Transition complex composite material La_2O_3 are relatively less ductile, they exhibit characteristics of high purity. Additionally, ductility increase is as we go on higher atomic No. in periodic table.

Furthermore, T_C demonstrates the highest ultrasonic velocities among the various pressure ranges indicating superior ductility at low pressure since attenuation $\alpha \propto V^3$, it is expected to reach its maxima

at low pressure. The minimal ultrasonic attenuation (UA) values for T_C further confirm the structural stability of its hexagonal phase.

6.5. Battery Application of La_2O_3

As we knew battery's are having two kind primary, battery and secondary battery in simple understanding the primary batteries are basic non rechargeable batteries which are generally med of Zn and Cu as working electrode which means cathode and anode and having a solid state $CuSO_4$ electrolyte. While on the other hand the secondary batteries are those which can be charged and discharged multiples time, and they uses semisolid galley form of polymer blended with transition type rare earth minerals complex like Li, Na, K, Mg etc. Which is called gal polymer electrolyte(GPE), this GPE is sandwiched in between two electrode one made with pure metal (like Aluminum, Steel, Silver, Cu or any transition metal like La etc.) which is called as cathode, and another electrode i.e. anode is med of activated carbon spin coated on graphene sheet. Now if we sandwiched our prepared GPE in between these electrodes like AC-cathode |GPE| metal-anode, this formation is called as supercapacitor, which is in general known as secondary rechargeable battery prototype.

Now in the cathode part which contains activated carbon (AC) on graphene, here AC are have micro diameter sized pores through which charged ions can passed while discharging from GPE to the AC further to the Graphene to complete the circuit which results an current flow in output network on the other hand in opposite side, on anode there are charge carries present initially in metallic which continuously going through the GPE while discharging, but normally in pure metal after a certain limit the supply of these ions to the GPE which further passes through the AC and Graphene is limited due to its porosity charge carrier concentration, and their temperature limits as in the case of primary batteries. But some how if we blend some composition in pure transition metal and increase its ion supply it can least longer time than usual after single charge, but imagine what if the charge carrier supply will rebuild in anode by reversing the direction of flow of charge which is not possible in primary because they are unidirectional and doesn't have pores to pass ions, now here if we look for our composition La_2O_3 this is a transition metal bounded with oxizon in lattice system due to the presence of negatively charged minral oxyzen the ion suply of this electrode is mutch high than the pure La electrode and this ions can be rebound with the La_2O_3 electode to make it, in ion saturated level as initialy, by reversing the directin of cahрге flow means by charging. here the come back charges are not fully 100% due to the basic factors like humidity ,temprature ,corosan,various kind of losses which includes phone-phone los and megnon-phonon los and their relaxation time to rebound with metal, this ration of charging and discharging is ingenral called as its C-Rate ,an higher value means long cyclic stabelity means we can charge our device multiples of time, and this C-rate is approximately 60-85% after fully discharging.here in this case of La_2O_3 there phone-phone and megnon-phonon los is keep decreasing up to near zero, which means at the higher pressure by using these transition composite anode we can assume our phone-phone and megnon-phonon los is to be negligible, which definitely results atleast smaller increment in our C-Rate i.e. a longer cycling period of charging and discharging, so as aresult we can say this La_2O_3 anode can be reliably used in batery industry.

7. Conclusions

Based on the comprehensive analysis of the HCP Transiton complex composit material La_2O_3 aresystem, the following conclusions have been drawn:

- The standard computational approach used to determine higher-order elastic coefficients for hexagonal nanomaterials, based on the Lennard-Jones potential model, has proven effective and applicable to the the HCP Transiton complex composit material La_2O_3 .

- The evaluated elastic properties confirm that the HCP Transion complex composit material La_2O_3 are Metal Compound are mechanically stable across all compositions.
- Young's modulus for these nanomaterials demonstrates greater anisotropy compared to the bulk modulus, as indicated by various anisotropy indices, suggesting direction-dependent mechanical behavior.
- The thermal relaxation time (τ) for all HCP Transion complex composit material La_2O_3 is found to be on the order of 10^{-13} seconds, supporting their classification as intermetallic nanomaterials. Notably, the minimum value of τ along the wave propagation direction at 850 implies the fastest phonon redistribution in this direction.
- G/B ratio, which is 0.9426 at STP confirms the Brittle nature of material
- The dominant contribution of p-p interactions to ultrasonic attenuation (U.A.) plays a key role in influencing the thermal conductivity of HCP Transion complex composit material La_2O_3 compound.
- Among all listed HCP Transion complex composit material La_2O_3 compound, Demonstrates superior mechanical properties, with stronger ionic bonding characteristics.
- The HCP Transion complex composit material La_2O_3 compound exhibit enhanced ductility, as evidenced by the lowest ultrasonic attenuation values.

This research could help in computational as well as non-destructive classification of nanomaterials. These findings serve as the basis for further research into the major thermo-physical properties of other nanomaterials. and also on the basis of above mentioned discussion on battery we can say this is an reliable source of anode in supercapecitor with improved C-rate.

Authors' Contributions

Vivek Chaurasiya: Conceptualization, Writing-original draft, Analyzing the results. Pramod Kumar Yadawa: Review, Visualization, Supervision.

Competing Interests

The authors declare that there are no conflicts of interest related to this work. There are no known competing financial interests or personal relationships that could have influenced the findings presented in this study.

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