Non-Linear Thermophysical Behaviour of Transition Metal Titanium

Ultrasonic properties reported for the first time

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PEER REVIEWED
Received 28th May 2022; Revised 28th September 2022; Accepted 7th October 2022; Online 10th October 2022

The propagation of ultrasonic waves in the hexagonal closed packed (hcp) structured lanthanide metal titanium has been investigated in the temperature range 300–1000 K. For this, initially the higher-order elastic constants (second-order elastic constants (SOECs) and third-order elastic constants (TOECs)) were computed using the Lennard-Jones interaction potential model. With the help of SOECs, other elastic moduli such as Young’s modulus (Y), bulk modulus (B), shear modulus (G), Poisson’s ratio (σ) and Pugh’s ratio (B/G) were computed using the Voigt-Reuss-Hill approximation. Three types of orientation-dependent ultrasonic velocities, including Debye average velocities, were evaluated using the calculated SOECs and density of titanium in the same temperature range. Thermophysical properties such as lattice thermal conductivity, thermal relaxation time, thermal energy density, specific heat at constant volume and acoustic coupling constant were evaluated under the same physical conditions. The ultrasonic attenuation due to phonon-phonon interaction is most significant under the chosen physical conditions. The ultrasonic properties of titanium are correlated with thermophysical properties to understand the microstructural features and nature of the material.

1. Introduction

The Group IV transition metals have drawn great interest both scientifically and technologically (1–3). The transition metals may have face-centred cubic (fcc) and body-centred cubic (bcc) structures as well as hcp structures at ambient temperature (2). Among these transition metals, titanium and its alloys attract attention from material scientists and researchers due to its low density, corrosion resistance and high strength for applications in various fields (4–6). Titanium has been alloyed with other elements such as iron, aluminium, vanadium and molybdenum to produce strong lightweight alloys for aerospace, military, industrial and automotive applications (7). In recent years, titanium has attracted attention as a biomaterial for artificial bones because of its biocompatibility (8). The phase transformations of titanium play a vital role in many manufacturing techniques and
the ability to control them is a means to achieve desired properties (9, 10).

First-principle computation has been extensively carried out to study the basic properties of materials, including the structural, elastic, mechanical and thermodynamic properties of transition metals (11–15). Several studies have reported ab initio calculations of the temperature dependence of elastic constants of transition metals within the quasi-static approach (16–23) and within the quasi-harmonic approximation (19, 21–23). Kun et al. described the electronic structure of transition metals using one-atom theory (23). The effect of pressure on the crystal structures of transition metals and their phase transformation has been studied by Xia et al. (24). Fisher et al. measured the elastic constants of titanium, zirconium and hafnium in the α-phase across a temperature range of 4–1155 K using an ultrasonic wave interference technique (25).

Besides these investigations, many theoretical studies have also been carried out into the effects of dopant element incorporation on the elastic properties of titanium (26–31). Argaman et al. used the quasi-harmonic approximation combined with phonon-based free energy calculation to investigate the dependence of elastic constants on temperature of hcp titanium (30). Song et al. have done a systematic study of the effect of doping in α-titanium clusters by second-row elements and first-row transition metals, focusing primarily on the calculation of the bulk modulus and energetics of dopant incorporation (27–29). Lobkis et al. reported that the ultrasonic properties of titanium-based alloys show a strong frequency-dependence of backscattering on the microstructure (31). Britton et al. managed to capture some elastic anisotropy of commercially pure titanium, but the range was smaller than expected compared to modulus measurements of single crystals (32). The orientation dependent elastic modulus and hardness have been reported by Kwon et al. (33).

The effect of ultrasonic vibration on microstructure evolution was investigated by Siu et al. (34).

Semiempirical interatomic potentials for hcp elements titanium and zirconium, based on the modified embedded-atom method formalism, have been developed by Kim et al. (35). The pressure-dependent mechanical and thermodynamic properties of fcc and bcc titanium have been explored by Zhang Yongmei et al. (36). Spreadborough et al. studied the measurement of the lattice expansions and Debye temperatures of titanium using X-ray methods (37). The elastic properties of the single-crystalline hexagonal phase of titanium was experimentally studied by Tane et al. at room temperature (38). However, the lack of information regarding the temperature-dependent elastic, mechanical, thermophysical and ultrasonic properties of titanium is the motivation for the present study.

Ultrasonic properties are an important way to characterise the microstructural features of materials. The ultrasonic attenuation is related to numerous physical quantities, such as higher order elastic constants, thermal conductivity, specific heat and thermal energy density which provide understanding of the solid-state behaviour of the materials. In the present manuscript, the temperature-dependent ultrasonic attenuation and nonlinear elastic and thermophysical properties of the metal titanium have been studied.

2. Computational Method

The higher-order elastic constants (SOECs and TOECs) are vital parameters as they are linked to a number of thermophysical aspects which help to understand the performance of condensed materials. To avoid the many complexities and approximations of a first principle calculation approach, the higher-order nonlinear elastic constants of titanium can be determined using a simple interaction potential model approach. Considering the Lennard-Jones potential as many body interactions potential, the SOECs and TOECs of a hexagonal wurtzite structured material can be calculated using the following expressions (39, 40):

\[
\begin{align*}
C_{11} &= 24.1 \rho^4 C' \\
C_{13} &= 1.925 \rho^4 C' \\
C_{44} &= 2.309 \rho^6 C' \\
C_{111} &= 126.9 \rho^2 B + 8.853 \rho^4 C' \\
C_{113} &= 1.924 \rho^2 B + 1.155 \rho^6 C' \\
C_{133} &= 3.695 \rho^6 B \\
C_{144} &= 2.309 \rho^6 B \\
C_{222} &= 101.039 \rho^2 B + 9.007 \rho^4 C' \\
C_{12} &= 5.918 \rho^4 C' \\
C_{33} &= 3.464 \rho^6 C' \\
C_{66} &= 9.851 \rho^6 C' \\
C_{112} &= 19.168 \rho^2 B - 1.61 \rho^4 C' \\
C_{123} &= 1.617 \rho^4 B - 1.155 \rho^6 C' \\
C_{155} &= 1.539 \rho^6 B \\
C_{244} &= 3.464 \rho^6 B \\
C_{333} &= 5.196 \rho^6 B
\end{align*}
\]
where \( p = c/a \) is axial ratio; \( B = \psi a^3/p^3 \); \( C' = \chi a/p^2 \); \( \chi = 1/8\{nb_0(n-m)/{a^{n+m}}\} \); \( \psi = -\psi/\{6a^2(m+n+6)\} \); and \( c \) is the height of the unit cell. The parameters (\( \chi \) and \( \psi \)) have been calculated using values of the unit cell parameter (\( a \)), axial ratio (\( p \)), the constant \( b_0 \) and positive integers (\( m, n \)).

Voigt, Reuss and Hill’s approaches have been used to calculate the bulk modulus (\( B \)), shear modulus (\( G \)) and Young’s modulus (\( Y \)) and are given by the following expressions (41, 42):

\[
\begin{align*}
M &= C_{11} + C_{12} + 2C_{33} - 4C_{13}; \\
B_R &= \frac{C^2}{M}; \\
G_Y &= \frac{M + 12(C_{44} + C_{66})}{30}; \\
Y &= \frac{9GB}{G + 3B}; \\
C^2 &= (C_{11} + C_{12})C_{33} - 4C_{13} + C^2_{13}; \\
B_Y &= \frac{2(C_{11} + C_{12}) + 4C_{13} + C_{31}}{9}; \\
G_R &= \frac{5C^2C_{44}C_{66}}{2[3B_Y C_{44} + C^2(C_{44} + C_{66})]}; \\
G &= \frac{G_Y + G_R}{2}; \\
\sigma &= \frac{3B - 2G}{2(3B + G)}.
\end{align*}
\]

The ultrasonic velocity and attenuation are the two dominant parameters required for the ultrasonic characterisation of a material. The ultrasonic velocity gives information about the mechanical, anisotropic and elastic properties of the medium through which it passes. The ultrasonic attenuation is the loss or absorption of ultrasonic energy by the medium through which it passes. It is representative of microstructural features of the material as it is related to several microstructural parameters through a number of mechanisms. At room temperature, due to the phonon-phonon (\( p-p \)) interaction, Akihieser loss and thermoelastic relaxation are two dominant processes of ultrasonic attenuation. The ultrasonic attenuation coefficient (\( \alpha_{abh} \)) due to phonon-phonon interaction (Mason approach) is given as (43, 44):

\[
\alpha_{abh} = 4c^2\Delta C_i/2\rho V^2 (1 + \omega^2 c^2)
\]

Here, \( \omega = 2\pi f \) is angular frequency of the wave; \( V \) is the velocity of longitudinal and shear wave; \( \Delta C \) is change in elastic modulus caused by strain and is given as:

\[
\Delta C = 3E_0 < (\gamma_j^3)^2 > -3 < \gamma_j^3 >^2 C_Y T
\]

where \( E_0 \) is the thermal energy density; \( \gamma_j \) are the Grüneisen numbers with \( j \)th direction of propagation and \( j \)th direction of polarisation of the wave. Mason used Grüneisen numbers \( < \gamma_j > \), which is directly related to the SOECs and TOECs (45). This approach is found to be very useful for the estimation of ultrasonic attenuation in various materials. Brügger (46) derived a formula for \( \gamma_j \) in the form of tensor notation as (45):

\[
-\gamma_j = -\gamma_j^k = U_j U_k + \frac{N_{pq} N_{qk}}{2C_{ij}} (C_{kjkq} + U_l U_s C_{jkprqs})
\]

where \( j, k \) are the two index symbols for strain; \( U_j \) and \( U_k \) are the direction cosine of the polarisation direction; \( N_{pq} \) and \( N_{qk} \) are the direction cosine of propagation direction; \( C' \) is the effective elastic modulus associated with wave propagation in this direction; \( C_{kjkq} \) and \( C_{jkprqs} \) are the SOECs and TOECs, respectively in tensor notation. Mason and other works introduced a non-linearity constant called the acoustic coupling constant, \( D \), which is defined as the measure of rate of conversion of acoustic energy into thermal energy and vice versa. \( D \) is calculated using \( < \gamma_j > \) and \( < \gamma_j^3 >^2 \) by the following expression:

\[
D = 9 < (\gamma_j)^2 > -3 < \gamma_j >^2 \frac{C_Y T}{E_0} = \frac{3\Delta C}{E_0}
\]

The time taken to re-establish equilibrium of the thermal phonons is called the thermal relaxation time (\( \tau \)) and is given by the following equation:

\[
\tau = \tau_S = \frac{\tau_L}{2} = \frac{3\chi}{C_Y V_D}
\]

Here, \( \tau_L \) and \( \tau_S \) are the thermal relaxation times for longitudinal and shear waves; and \( C_Y \) are the thermal conductivity and specific heat per unit volume of the material; and \( V_D \) is the Debye average velocity given by the following equation (45, 47):

\[
V_D = \left[ \frac{1}{3} \left( \frac{1}{V_L^2} + \frac{1}{V_S^2} + \frac{1}{V_T^2} \right) \right]^{-1/3}
\]

where
In the above equations, \( V_1, V_2 \) and \( V_3 \) are the velocities of longitudinal, quasi-shear and shear waves, respectively; \( \rho \) and \( \theta \) are the density of the material and angle with the unique axis (z-axis) of the crystal respectively.

The thermal conductivity of a condensed material is one of its most vital physical parameters. At a fundamental level, the study of the underlying physics of heat conduction has provided a deep and detailed understanding of the nature of lattice vibrations in solids. The lattice thermal conductivity (\( \kappa \)) of the material is computed using the method described by Slack and Morelli (48) and is given by the following equation:

\[
\kappa = A \frac{\rho \delta^3}{<|v|>^2 Tn^{2/3}}
\]

where \( \delta \) is the atomic mass of the atom; \( <|v|> \) is the Grüneisen number; \( A \) is a constant; and \( \theta_0 \) is the Debye temperature. The formulae for \( A \) and \( \theta_0 \) are given by:

\[
A = \frac{2.43 \times 10^{-8}}{1 - 0.514/<|v|> + 0.228/<|v|>^2}
\]

\[
\theta_0 = \frac{h V_D}{K_B} \left[ \frac{3n(N_A \rho)}{4\pi \left( \frac{\rho^2}{M} \right)^2} \right]^{1/3}
\]

where \( n \) is the number of atoms per molecule; \( \rho \) is the material density; \( N_A \) is Avogadro’s number; \( K_B \) is Boltzmann’s constant; \( V_D \) is the Debye average velocity; and \( h \) is reduced-order Planck’s constant.

The propagation of a longitudinal wave creates compression and rarefaction throughout the lattice. The rarefied regions are colder than the compressed regions. Thus, there is a flow of heat between these two regions which results in thermoelastic loss. The thermoelastic loss is given by the following equation (49, 50):

\[
(z/\rho^2)_\text{th} = 4\pi^2 <|v|>^2 \kappa T/2\rho V_1^5
\]

The thermoelastic loss for the shear wave has no physical significance because the average of the Grüneisen number for each mode and direction of propagation is equal to zero for the shear wave. Only the longitudinal wave is responsible for thermoelastic loss because it causes variation in entropy along the direction of propagation. The total ultrasonic attenuation is given by the following equation (39, 45):

\[
(z/\rho^2)_{\text{total}} = (z/\rho^2)_\text{th} + (z/\rho^2)_L + (z/\rho^2)_S
\]

where \( (z/\rho^2)_L \) and \( (z/\rho^2)_S \) are the ultrasonic attenuation coefficients over frequency squared for the longitudinal and shear waves due to p-p interactions only.

3. Results and Discussion

The basal plane parameter \( (a) \) and axial ratio \( (p) \) for metal titanium were taken from the literature (8). The values of \( m \) and \( n \) for titanium are taken as 6 and 7 respectively. The value of the Lennard Jones parameter \( (b_0) \) determined under equilibrium conditions for titanium is \( 0.664 \times 10^{-64} \text{ erg cm}^2 \).

SOECs and TOECs for the hcp structured metal titanium in temperature range 300–1000 K have been calculated using Equation (i). The calculated values of SOECs and TOECs are presented in Figure 1 and Figure 2 respectively.

Elastic constants represent the elastic behaviour of materials and offer significant information regarding the bonding characteristics, anisotropy and hardness. The mechanical properties of the materials can also be analysed using knowledge of the elastic constants. It is obvious from Figure 1 that the calculated values of elastic constants decrease with temperature. This is because as the temperature increases, the interatomic distances between the atoms change and thus the potential interactions, which lead to decrease in the elastic constants. The temperature-dependent elastic constants are essential parameters for understanding the effect of temperature on the stiffness and mechanical strength of materials. It is also obvious from Figure 1 that the obtained values of SOECs are approximately similar to the experimentally reported values of Ogi et al. (51). At 300 K, the calculated values of \( C_{11}, C_{12}, C_{33} \) and \( C_{44} \) differ by 3.86\%, 13.59\%, 8.04\% and 8.67\% while the maximum deviation in \( C_{66} \) is 22.36\%. At a higher temperature regime, the values are quite similar to all the SOECs. There is a slight difference from the reported results because in the present model we have considered the interaction up to the second nearest neighbours. The comparison of \( C_{13} \) with the experimental data has not been done due to a lack of reported data in the literature.

For the hcp structured materials, the Born structural stability criteria for a crystal lattice are as follows (42, 52): \( C_{44} > 0 \); \( C_{11} > C_{12} \); \( (C_{11} + 2C_{12}) C_{33} > 2C_{13}^2 \). It is obvious from Figure 1 that titanium follows Born’s conditions for mechanical stability. Therefore, metal titanium is mechanically...
stable. Also, these elastic constants are intimately interrelated to various mechanical properties, such as bulk modulus ($B$), shear modulus ($G$), Young’s modulus ($Y$), Poisson’s ratio ($\sigma$) and Pugh’s ratio ($P$). The bulk modulus is a parameter that can resist deformation in terms of the volume strain under applied pressure or temperature. The shear modulus is a valid index of the elastic properties for examining the changes in shape under transverse internal forces. Young’s modulus is the stiffness of a material at the elastic stage of the tensile test. These elastic moduli $B$, $G$, $Y$, $\sigma$ and $P$ are presented in Table I. It is obvious from Table I that the calculated value of all the elastic moduli decreases with increases in temperature. At room temperature, the calculated values of
that the values of TOECs are negative. The negative values of the TOECs indicate negative strain in the crystals. However, the TOECs at room temperature show good agreement between our present study and our earlier reported study (53). Also, the values of TOECs are well matched with the same group transition metal hafnium (54). All the values of TOECs are negative as reported in other hcp structured materials like gallium nitride, gallium arsenide, zinc sulfide and magnesium diboride (44, 47, 49, 55). These comparisons justify our calculation of SOECs and TOECs.

The anharmonic properties of crystalline materials can be understood by knowledge of the Grüneisen parameter. It is the measurement of change in the vibrational frequency of atoms of crystalline materials with a change in volume. This parameter is directly proportional to SOECs and TOECs and inversely proportional to the specific heat and density of the material. We have computed the Grüneisen parameters following the procedure used in our previous work (45). The evaluated values are presented in Table II.

It is obvious from Table II that the values of Grüneisen’s parameters decrease gradually with temperature. These parameters are useful to estimate thermal conductivity as well as ultrasonic attenuation. The elastic constants of the materials are also related to fundamental solid-state phenomena such as Debye temperature, specific heat and energy density. The specific heat at constant volume ($C_V$) and energy density ($E_0$) were evaluated using the table of $\theta_D/T$ (where $\theta_D$ is Debye temperature) given in the American Institute of Physics (AIP) Handbook (56). The calculated thermophysical quantities thermal conductivity ($k$), $C_V$, $E_0$ and thermal relaxation time ($\tau$) are shown in Figure 3.

The thermal conductivity is proportional to the temperature and inversely proportional to the square of the Grüneisen parameter. It is clear from Figure 3(a) that the thermal conductivity of titanium decreases with temperature despite the slight decay in the Grüneisen parameter. At low temperatures, the phonons have a very long wavelengths and are scattered primarily by the crystal boundaries. In this regime, scattering is
frequency- and temperature-independent and the thermal conductivity is dependent on the specific heat. At higher temperatures, anharmonic phonon interaction dominates. The probability of these anharmonic scattering events increases as the temperature increases so that the thermal conductivity goes through the maximum and then decreases. The anharmonic interactions are usually three-phonon processes in which two phonons collide and create a third or one phonon breaks into two phonons. As the temperature of the crystal increases, the mean energy of the dominant phonons increases and the three-phonon scattering processes become most probable. It is also clear that in the three-phonon process, momentum is conserved in the sense that the algebraic sum of all phonon wave vectors is zero and is least affected by anharmonicity caused by four-phonons interaction mechanism occurring at high enough temperature. Unfortunately, to the best of our knowledge, no previous experimental data regarding the thermal conductivity of titanium have been reported to allow direct comparisons. However, the order and nature of thermal conductivity are quite similar to experimentally reported data of zirconium (57). It is obvious from Figure 3(b) that the thermal relaxation time decreases non-linearly with temperature and resembles the same characteristics of thermal conductivity. Therefore, both the thermal conductivity and thermal relaxation time are least affected by the Grüneisen’s parameter or anharmonicity of the metal titanium in a given temperature range. The thermal relaxation for the chosen metal titanium is of the order of picoseconds which is comparable to that for previously reported hcp structured crystals.

Ultrasonic velocities (longitudinal, \(V_L\); shear, \(V_S\); and Debye average velocity, \(V_D\), acoustic coupling constants \((\alpha)\) and the total ultrasonic attenuation over frequency square \((\alpha f^2)_{\text{total}}\) for titanium are displayed in Table III.

Table III indicates that the ultrasonic velocities along with Debye average velocity in titanium decrease with temperature, which is caused by a decrease in SOEC with temperature. It is also clear from Table III that the acoustic coupling constant of titanium for longitudinal and shear waves has an approximately constant value. Thus, it might be predicted that the amount of ultrasonic energy converted in the form of thermal energy at high temperatures for titanium will be approximately the same. The calculated orientation-dependent ultrasonic wave velocities and Debye average velocity in the temperature range 300–1000 K are shown in Figure 4.

Figure 4 shows that the velocities \(V_L\) and \(V_S\) have minima and maxima at 35° and 45° respectively with the unique axis of the crystal while \(V_D\) increases with the angle from the unique axis. The variation of the angle-dependent velocity curves in the present work is found to be close to that for Laves phase compounds and hexagonal wurtzite structured materials (gallium nitride, aluminium nitride, indium nitride, cadmium sulfide and cadmium selenide) (58–60). Thus, the computed velocities for titanium are justified. It is obvious from Figure 4(d) that the Debye average velocity, \(V_D\), for titanium increases with the angle, with maxima at 55° in the temperature range 300–1000 K. Since \(V_D\) is calculated with the help of \(V_L\), \(V_S\) and \(V_D\) using Equation (vi) and (ix), the angle variation of \(V_D\) is influenced by the constituent ultrasonic velocities. The maximum \(V_D\) at 55° is due to a significant hump in longitudinal and pure shear wave velocities and a decrease in quasi-shear wave velocity.

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**Table II Average of Grüneisen Number for Longitudinal Wave \(\langle \gamma_L \rangle\), Average of Square of Grüneisen Number for Longitudinal Wave \(\langle \gamma^2_L \rangle\) and Shear Wave \(\langle \gamma^2_S \rangle\), of Metal Titanium in Temperature Range 300–1000 K**

<table>
<thead>
<tr>
<th>(T, K)</th>
<th>(\langle \gamma \rangle)</th>
<th>(\langle \gamma^2 \rangle_L)</th>
<th>(\langle \gamma^2 \rangle_S)</th>
</tr>
</thead>
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<td>300</td>
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<td>0.4697</td>
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Fig. 3. (a) Thermal conductivity; (b) thermal relaxation time; (c) specific heat capacity; and (d) thermal energy density of metal titanium in temperature range 300–1000 K

<table>
<thead>
<tr>
<th>$T$, K</th>
<th>$V_L \times 10^3$ m s$^{-1}$</th>
<th>$V_S \times 10^3$ m s$^{-1}$</th>
<th>$V_D \times 10^3$ m s$^{-1}$</th>
<th>$D_L$</th>
<th>$D_S$</th>
<th>$(\alpha/f^2)_{total} \times 10^{-17}$ Nps$^2$ m$^{-1}$</th>
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<tr>
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<td>56.830</td>
<td>1.323</td>
<td>742.628</td>
</tr>
<tr>
<td>950</td>
<td>5.804</td>
<td>2.983</td>
<td>3.299</td>
<td>56.848</td>
<td>1.33</td>
<td>818.312</td>
</tr>
<tr>
<td>1000</td>
<td>5.784</td>
<td>2.976</td>
<td>3.291</td>
<td>56.867</td>
<td>1.337</td>
<td>895.317</td>
</tr>
</tbody>
</table>
It can be concluded that the average sound wave velocity is maximum for a sound wave traveling at 55° with respect to the unique axis of the crystal. The orientation dependent calculated thermal relaxation time is displayed in Figure 5.

The angle-dependent thermal relaxation time curves follow the reciprocal nature of $V_D$. Thermal relaxation time ($\tau$) has a maximum value of 2.703 ps for wave propagation along the unique axis $\theta = 0^\circ$ of titanium at room temperature and a minimum value of $\tau$ for titanium is found to be 2.119 ps along $\theta = 55^\circ$ at 600 K. The evaluated value of $\tau$ in the order of picoseconds confirms the metallic phase of titanium at the chosen temperature regime (61). For wave propagation, the lowest thermal relaxation time along $\theta = 55^\circ$ infers that the re-establishment time for equilibrium distribution of thermal phonons will be minimum.
the evaluation of ultrasonic attenuation, it has been assumed that the wave is propagating along the unique axis <001> direction of the chosen metal titanium. The ultrasonic attenuation coefficient over frequency square for the longitudinal and shear waves has been calculated using Equation (iii) under the condition \( \omega \tau << 1 \) and the thermoelastic loss over frequency square \( \alpha / f^2 \) has been calculated with the Equation (xiii) and displayed in Figure 6.

In the calculation of ultrasonic attenuation, it is assumed that the ultrasonic wave is propagating along the unique axis \( \theta = 0^\circ \) of the material. As the temperature increases, a significant decrease in thermal conduction is observed due to the scattering of phonons. It can be seen from Figure 6 that as the temperature increases, the Akhieser loss has a dominant effect on the total ultrasonic attenuation because the anharmonic interaction between acoustic and thermal phonons increases with temperature. Total ultrasonic attenuation over frequency squared increases with temperature despite the anomalous behaviour in thermal conductivity because of the dominant effect of energy density which increases at the same time. The ultrasonic attenuation of the longitudinal mode has been found to be higher than that of the shear mode because of the larger acoustic coupling constant value for the longitudinal mode \( D_L \), compared with the shear mode \( D_S \). Ultrasonic attenuation due to the shear wave is greater than that due to the longitudinal wave, which can be attributed to the smaller value of \( C_{44} \) compared with \( C_{11} \) and this affects the wave propagation in the medium. Unfortunately, to the best of our knowledge, no previous experimental or theoretical data regarding ultrasonic attenuations have been reported previously to allow direct comparisons.

4. Conclusions

The theory for higher-order elastic constants is well validated for hcp structured metal titanium in the temperature range 300–1000 K. The computed SOECs, TOECs, ultrasonic velocities and elastic moduli of titanium are in excellent agreement with previous reported theoretical and experimental results which confirms the accuracy and feasibility of the computational method. Combined with the brittle/ductile criteria, the results obtained from the evaluation of Poisson’s ratio and Pugh’s index indicate that titanium behaves like a brittle material. The evaluated value of thermal relaxation time for titanium is of the order of picoseconds, which validates the metallic phase of titanium in the chosen temperature range 300–1000 K. For wave propagation, the re-establishment time for equilibrium distribution of thermal phonons must be minimum for propagation of a wave along \( \theta = 55^\circ \). The acoustic coupling constant of titanium for a longitudinal wave is approximately five times larger than nitrides of gallium, indium and aluminium. As a result, the conversion of acoustic energy into thermal energy will be considerable for titanium. Anharmonic interactions are the principal mechanism responsible for ultrasonic attenuation in titanium. The acoustic coupling constant and thermal conductivity are the dominant factors for total ultrasonic attenuation. The results obtained in the present investigations may be useful for future studies and industrial applications.

Acknowledgements

The authors are extremely thankful to the U.G.C., New Delhi and the U.P. Higher Education Council Board, Lucknow for the financial support.

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