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Investigation of zirconium nanowire by elastic, thermal and ultrasonic analysis

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Abstract: The elastic, thermal and ultrasonic properties of zirconium nanowire (Zr-NW) have been investigated at room temperature. The second and third order elastic constants (SOECs and TOECs) of Zr-NW have been figured out using the Lennard–Jones Potential model. SOECs have been used to find out the Young’s modulus, bulk modulus, shear modulus, Poisson’s ratio, Pugh’s ratio, Zener anisotropic factor and ultrasonic velocities. Further these associated parameters of Zr-NW have been utilized for the evaluation of the Grüneisen parameters, thermal conductivity, thermal relaxation time, acoustic coupling constants and ultrasonic attenuation. On the basis of the above analyzed properties of Zr-NW, some characteristics features of the chosen nanowire connected with ultrasonic and thermo-physical parameters have been discussed.

Keywords: elastic constants; thermal conductivity; ultrasonic attenuation; Zirconium nanowire.

1 Introduction

Researchers and material scientists are always excited to discover advanced materials with exotic properties which can extrude to the old conventional materials. The

development of nanotechnology in earlier phase gives the potential benefits to the material science. Nowadays, nanoscience has become one of the most stimulating forces to influence the interdisciplinary science and technology. The investigations in these areas begin with the understanding of material’s behaviour at nanoscale. The attempts were done to control over the crucial physical properties of the materials such as conductivity, capacity, strength, ductility, reactivity etc. in different combination of the matters. This will result in the enhancement of the material’s performance at ambient physical conditions. When the size or dimension of a material is continuously reduced from a large or macroscopic size to a size up to 100 nm, the properties remain the same but below 100 nm, dramatic changes in properties can occur [1]. Thus, the bulk properties of the materials become modified when their sizes are reduced to the nano range (1–100 nm). If one dimension is reduced to the nano-range, keeping other two dimensions unchanged, we obtain a structure known as a ‘quantum well’. If two dimensions are reduced and one remains unchanged, the resulting structure is referred as a ‘nanowire’. The single crystalline NWs are considered as the imperative division of the nanostructure materials due to its superior properties. Currently, the magnetic NWs have drawn considerable interest of researchers worldwide due to their applications in the high-density magnetic storage media, giant magnetoresistance (GMR) sensors [1, 2], bio-magnetic [3], medical devices [4], etc. Among the magnetic nanowires, Zirconium nanowires (Zr-NWs) are widely studied material for its two unusual properties. The first one is the temperature induced phase transformation and the second one is the plastic deformation by twinning. Zr-NWs are the phase changing material and exist in hexagonal close packed (HCP) phase at room temperature (300 K) [5]. Figure 1 shows the HCP structure of the Zr nanowire and its cross-sectional view. Figure 1 clearly indicates that very few Zr atoms are lying on the surface of nanowire in comparison to the volume.

In the field of non-destructive characterization, the ultrasonic non-destructive technique (NDT) has been the most extensively used for the characterization of the materials. The structural inhomogeneities, non-linear elastic properties, phase transformations, electrical properties,

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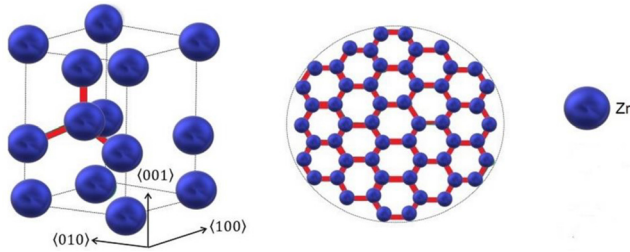


Figure 1: HCP structure of the Zr nanowire and its cross-sectional view.

dislocations, grains, thermal properties, size of particles in nanostructured materials, vacancies in the lattice sites in the materials are well related to the ultrasonic attenuation and velocity [6–8]. The ultrasonic studies at nanoscale are rarely found in the literature. Only some scarce investigations have been reported in the available literature [9, 10]. Hu et al. [11] created embedded atom method (EAM)-type many-body potentials for the HCP metals. These potentials reproduce for each metal considered the experimentally observed equilibrium density, c/a ratio, cohesive energy, second-order elastic constants (SOECs) and the vacancy formation energy. A modification term has been also introduced for describing metals with negative Cauchy pressure. Finnis–Sinclair (F-S) type many-body potentials have been applied for the HCP metals: Co, Zr, Ti, Ru, Hf, Zn, Mg and Be by Igarashi et al. [4]. They found that each of the potentials has been represented by a stable HCP lattice with a particular non-ideal c/a ratio.

As per our knowledge, no one has studied the Zr-NW for its mechanical, thermal and acoustical properties. These lacks of information motivated us to study these additional properties of the Zr-NW. In present investigation, first of all, we computed the SOECs and TOECs for Zr-NW using Lennard–Jones potential. The obtained values of SOECs have been applied to find out the Young’s modulus, bulk modulus, shear modulus, Poisson’s ratio, Zener anisotropic factor, ultrasonic velocities and thermal conductivity. Further, these evaluated parameters have been used to find out thermal relaxation time, acoustic coupling constants and ultrasonic attenuation due to phonon–phonon (p-p) interaction and thermal relaxation mechanisms. Obtained results have been presented, compared, and discussed with available findings of Zr and other reported similar nanowires at room temperature.

2 Computational method

There are various methods to calculate the elastic constants of the condensed materials. Among this first

principle method based on density functional theory (DFT) within the generalized gradient approximation (GGA) and quasi-harmonic approximation (QHA) are mostly used for calculation of elastic constants [12, 13]. In these DFT theories, there are many approximations for the estimation of higher order elastic constants. The interaction potential model approach is also one of the best-established theories for the determination of higher order elastic constants of HCP and hexagonal wurtzite structured materials [14–16]. In this work, interaction potential model approach has been used for the calculation of higher order elastic constants. The formulations of higher order elastic constants have been obtained by the second or third order strain derivative of elastic energy density.

A generalized definition of n th order elastic constant is the partial derivatives of the thermodynamic potential of the medium subjected to finite deformation and mathematically given by following expression as [17, 18]:

$$C_{ijklmn\dots} = \frac{\partial^n F}{\partial \eta_{ij} \partial \eta_{kl} \partial \eta_{mn} \dots} \quad (1)$$

where, F and η_{ij} represent free energy density and Lagrangian strain component tensor respectively. F can be expanded in terms of strain η using Taylor series expansion as:

$$F = \sum_{n=0}^{\infty} F_n = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\partial^n F}{\partial \eta_{ij} \partial \eta_{kl} \partial \eta_{mn} \dots} \right) \eta_{ij} \eta_{kl} \eta_{mn} \dots \quad (2)$$

Thus the free energy density upto cubic term is written as:

$$F_2 + F_3 = \frac{1}{2!} C_{ijkl} \eta_{ij} \eta_{kl} + \frac{1}{3!} C_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn} \quad (3)$$

For HCP material the basis vectors are $a_1 = a \left(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0 \right)$, $a_2 = a (0, 1, 0)$ and $a_3 = a (0, 0, c)$ in Cartesian system axes. Here a and c are the unit cell parameters. The unit cell of HCP material consists of two nonequivalent atoms: six atoms in basal plane and three-three atoms above and below the basal plane. Thus both first and second neighbourhood consists of six atoms. The $r_1 = a (0, 0, 0)$ and $r_2 = \left(\frac{a}{2\sqrt{3}}, \frac{a}{2}, \frac{c}{2} \right)$ are the position vectors of these two type of atoms.

The potential energy per unit cell up to second nearest neighbour is written as follows:

$$U_2 + U_3 = \sum_{I=1}^6 U(r_I) + \sum_{J=1}^6 U(r_J) \quad (4)$$

where, I refer to atoms in the basal plane and J refers to atoms above and below the basal plane. When the crystal is deformed homogeneously then interatomic vectors in undeformed state (r) and deformed state (r') are related as:

$$(r')^2 - (r)^2 = 2\varepsilon_i \varepsilon_j \eta_{ij} = 2\Theta \quad (5)$$

where, ε_i and ε_j are the Cartesian component of vector r . The energy density U can be explained in terms of Θ as [19, 20]:

$$U_n = (2V_c)^{-1} \sum \frac{1}{n!} \Theta^n D^n \phi(r) \quad (6)$$

Using Eqs. (4) and (6), the energy density U involving cubic terms can be written as:

$$U_2 + U_3 = (2V_c)^{-1} \left[\sum_{i=1}^6 \frac{1}{2!} \Theta_i^2 D^2 \phi(r_i) + \sum_{j=1}^6 \frac{1}{2!} \Theta_j^2 D^2 \phi(r_j) \right] + (2V_c)^{-1} \left[\sum_{i=1}^6 \frac{1}{3!} \Theta_i^3 D^3 \phi(r_i) + \sum_{j=1}^6 \frac{1}{3!} \Theta_j^3 D^3 \phi(r_j) \right] \quad (7)$$

where, $V_c = [3^{1/2}/2] a^2 c$ stands for the volume of the elementary cell, $D = R^{-1}d/dR$ and $\phi(r)$ is the interaction potential. The energy density is considered to be function of Lennard Jones potential (many body interactions potential) and given as [21, 22]:

$$\phi(r) = -\frac{a_0}{r^m} + \frac{b_0}{r^n} \quad (8)$$

where, a_0, b_0 are constants; m, n are integers and r is the distance between atoms. The interaction considered up to second nearest neighbours. Developing the interaction potential model leads to calculate 6 SOECs and 10 TOECs of the HCP material and can be written as the following set of equations [19–22]:

$$\left. \begin{array}{ll} C_{11} = 24.1p^4C' & C_{12} = 5.918p^4C'' \\ C_{13} = 1.925p^6C'' & C_{33} = 3.464p^8C'' \\ C_{44} = 2.309p^4C'' & C_{66} = 9.851p^4C'' \\ C_{111} = 126.9p^2B + 8.853p^4C'' & C_{112} = 19.168p^2B - 1.61p^4C'' \\ C_{113} = 1.924p^4B + 1.155p^6C'' & C_{123} = 1.617p^4B - 1.155p^6C'' \\ C_{133} = 3.695p^6B & C_{155} = 1.539p^4B \\ C_{144} = 2.309p^4B & C_{344} = 3.464p^6B \\ C_{222} = 101.039p^2B + 9.007p^4C' & C_{333} = 5.196p^6B \end{array} \right\} \quad (9)$$

where, $p = c/a$: axial ratio; $C' = \chi a/p^5$; $B = \psi a^3/p^3$. In present study, we have expanded the theory for theoretical evaluation of parameters χ and ψ . The potential energy can

be expanded in the powers of changes in the squares of distances. The expansion up to cubic term can be written as:

$$\phi = \phi_0 + \psi \sum_{i=1}^2 [\Delta r_i^2]^2 + \chi \sum_{i=1}^2 [\Delta r_i^2]^3 \quad (10)$$

According to Eq. (4), χ and ψ can be expressed as:

$$\chi = \frac{1}{2!} \left[\frac{d^2 \phi(r)}{d(r^2)^2} \right] \quad (11)$$

$$\psi = \frac{1}{3!} \left[\frac{d^3 \phi(r)}{d(r^2)^3} \right] \quad (12)$$

By solving Eqs. (11) and (12) for HCP materials we have:

$$\chi = (1/8) [\{nb_0(n-m)\}/\{a^{n+4}\}] \quad (13)$$

$$\psi = -\chi/\{6a^2(m+n+6)\} \quad (14)$$

The χ and ψ can be computed using Eqs. (13) and (14) and appropriate values of m, n and b_0 . In our approach very few parameters (lattice parameters) are required for the evaluation of higher order elastic constants. Also, there are fewer approximations in comparison to first principle calculation and gives the good results; hence, this approach is better than the other models.

Calculation of shear modulus (G) and bulk modulus (B) have been done using Voigt and Reuss's approaches [23, 24]. The approximations of uniform stress and uniform strain have been used in the Voigt and Reuss's approaches, respectively. Further, Under Hill's methods, average values of the both approaches have been used to calculate the resultant values of B and G [24]. Young's modulus (Y) and Poisson's ratio (σ) are

determined using the values of B and G [25, 26]. Following expressions (Eq. (15)) have been used for the calculation of Y, B, G , and σ .

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

The mechanical and anisotropic properties of condensed materials are well related with ultrasonic velocity because the velocity of ultrasonic wave is mainly depends upon the SOECs and density. On the basis of mode of vibration, there are three types of ultrasonic velocities in HCP structured materials. One longitudinal V_1 and two shear (V_2 , V_3) waves velocities. The velocities of ultrasonic wave as a function of angle between direction of propagation and unique axis for HCP structured materials are given by following set of equations:

where f stands for the frequency of the ultrasonic wave; V is the velocity of ultrasonic wave and E_0 is the thermal energy density. The measure of conversion of acoustical energy into thermal energy is known as acoustical coupling constants, denoted by D , and is given by following expression:

$$D = 3 \left(3E_0 \langle \gamma_i^j \rangle^2 - \langle \gamma_i^j \rangle^2 C_V T \right) / E_0 \quad (19)$$

where C_V is the specific heat per unit volume of the material, T is the temperature and γ_i^j is the Grüneisen number; i

$$\left. \begin{aligned} V_1^2 &= \left\{ C_{33} \cos^2 \theta + C_{11} \sin^2 \theta + C_{44} + \left\{ [C_{11} \sin^2 \theta - C_{33} \cos^2 \theta + C_{44} (\cos^2 \theta - \sin^2 \theta)]^2 \right. \right. \\ &\quad \left. \left. + 4 \cos^2 \theta \sin^2 \theta (C_{13} + C_{44})^2 \right\}^{1/2} \right\} / 2\rho \\ V_2^2 &= \left\{ C_{33} \cos^2 \theta + C_{11} \sin^2 \theta + C_{44} - \left\{ [C_{11} \sin^2 \theta - C_{33} \cos^2 \theta + C_{44} (\cos^2 \theta - \sin^2 \theta)]^2 \right. \right. \\ &\quad \left. \left. + 4 \cos^2 \theta \sin^2 \theta (C_{13} + C_{44})^2 \right\}^{1/2} \right\} / 2\rho \\ V_3^2 &= \{ C_{44} \cos^2 \theta + C_{66} \sin^2 \theta \} / \rho \end{aligned} \right\} \quad (16)$$

where, V_1 , V_2 , and V_3 are the longitudinal, quasi-shear, and shear wave velocities; ρ and θ are the density of the material and angle with the unique axis (z -axis) of the crystal respectively. For hexagonal structured crystal the Debye average velocity along any angle with the unique axis is given by the equation as [19, 20]:

$$V_D = \left[\frac{1}{3} \left(\frac{1}{V_1^3} + \frac{1}{V_2^3} + \frac{1}{V_3^3} \right) \right]^{-1/3} \quad (17)$$

At higher temperature, phonon-phonon interaction (Akhieser's type loss) and thermoelastic loss are the two dominating processes which are appreciable for attenuation of ultrasonic wave. The attenuation due to Akhieser's loss is given by the following equation:

$$(\alpha/f^2)_{Akh} = \frac{4\pi^2 \tau E_0 (D/3)}{2\rho V^3} \quad (18)$$

and j are the mode and direction of the propagation. When the ultrasonic waves propagate through the material, the equilibrium of lattice phonon distribution gets disturbed. The time takes for re-establishment of equilibrium of the thermal phonons is named as thermal relaxation time, denoted by τ , and is given by following expression [14]:

$$\tau = \tau_s = \tau_L / 2 = \frac{3k}{C_V V_D^2} \quad (20)$$

where the thermal relaxation time for the longitudinal wave and shear wave are represented by τ_L and τ_s respectively, k is the thermal conductivity of the material. The thermoelastic loss $(\alpha/f^2)_{Th}$ is calculated using the following equation [9, 10]:

$$(\alpha/f^2)_{Th} = 4\pi^2 \langle \gamma_i^j \rangle^2 \frac{kT}{2\rho V_L^5} \quad (21)$$

The total attenuation is given by the following equation as:

$$(\alpha/f^2)_{Total} = (\alpha/f^2)_{Th} + (\alpha/f^2)_L + (\alpha/f^2)_S \quad (22)$$

where $(\alpha/f^2)_{Th}$ is the thermoelastic loss, $(\alpha/f^2)_L$ and $(\alpha/f^2)_S$ are the ultrasonic attenuation coefficient for the longitudinal wave and shear wave respectively. All the computation of required parameters has been done manually as well as C++ language program.

3 Results and discussion

The lattice parameter ($a = 3.23$) and axial ratio ($p = 1.59$) for the Zr-NW at room temperature (300 K) is taken from literature [2]. The calculated values of Lennard-Jones parameter (b_0) for the chosen material evaluated under equilibrium condition is 1.7764×10^{-65} erg-cm⁷. For structured material (face centred cubic, body-centred cubic, or hexagonal close-packed) the values of exponents' m and n can have values 6 and 12, 6 and 9, 6 and 7 depending upon structure or long/short range of interaction [27, 28]. In present work, we have chosen all possible combinations of m and n (6 and 12, 6 and 9, 6 and 7) for calculation of elastic constants. It has been found that, if we just change the value of m and n (rather than 6 and 7) in the calculations of elastic constants, absurd order of elastic constants have been found. Therefore we have used $m = 6$ and $n = 7$, for the calculation of second and third order elastic constants of Zr-NW at room temperature. The calculated values of SOECs and TOECs for chosen material at room temperature and other elastic moduli (Young's modulus (Y), bulk modulus (B), shear modulus (G), Poisson's ratio (σ) and Zener anisotropic factor (Z_A)) which have been evaluated with the help of calculated value of the SOECs using Eq. (15). These calculated values are presented in Table 1.

The SOECs have been used for the determination of the ultrasonic attenuation, ultrasonic velocity and other related parameters. It is clear from Table 1 all the calculated value of SOECs for Zr-NW have been found nearly

close with previous value reported by Hu et al. [11]. The comparison shows that all these calculated values of SOECs are in good agreement with previous predictions. The slightly difference is because of we considered the interaction in present approach up to second nearest neighbours. The hardness, compressibility, ductileness, brittleness, toughness, and bonding nature of the material are also well correlated with the SOECs. For a stable HCP structure, the five independent SOECs should satisfy the distinguished Born stability criteria [25, 26] i.e., $C_{11} - |C_{12}| > 0$, $(C_{11} + C_{12}) C_{33} - 2C_{13}^2 > 0$ and $C_{44} > 0$. It is obvious from Table 1, Zr-NW is mechanically stable because all the values of SOECs are positive and satisfy the Born's mechanical stability constraints. Pugh's ratio (B/G) and Poisson's ratio (σ) define brittleness and ductility of a solid. A solid is usually brittle in nature with $\sigma \leq 0.26$ and $B/G \leq 1.75$; otherwise it is ductile in nature [26, 29]. In this evaluation, the higher values of Poisson's and Pugh's ratio with respect to their critical values indicate that Zr-NW have ductile in nature at room temperature. The Zener anisotropic ratio (Z_A) deviates from the unity, which settles the anisotropic behaviour of Zr-NW at room temperature. Therefore, all the mechanical behaviour of a material can be described by the knowledge of these elastic moduli.

TOECs are important parameters for the knowledge of anharmonic properties of the materials. The calculated value of TOECs could not be compared due to lack of data reported in various literatures. The values of TOECs is negative that can be reported in other HCP structured material like third group nitrides, HfX_2 (S, Se), GaAs NWs, Lave phase compounds, ZrX_2 (S, Se), and ZnS [14–16, 19–21]. The negative values of TOECs indicate the negative strain in the crystals. Hence, our theoretical approach for the calculation of non-linear higher order elastic constants for HCP structured Zr-NW is justified and validated. The mechanical and anisotropic behaviour of the materials have been associated with ultrasonic velocity. The angle dependent ultrasonic velocities of Zr-NW have been computed using Eq. (16). The variations of ultrasonic velocities vs angle are shown in Figure 2.

Table 1: SOECs (in GPa), B (in GPa), G (in GPa), Y (in GPa), σ , Z_A , and TOECs (in GPa) of Zr-NW at room temperature.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B	G	σ	Z_A
Present	190.45	74.44	61.30	175.24	46.20	77.84	105.14	58.33	0.26	0.76
Ref. [11]	144.00	74.00	67.00	166.00	33.40	–	–	–	–	–
C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{344}	C_{144}	C_{155}	C_{222}	C_{333}	
–3105.6	–49.23	–98.81	–125.58	–592.96	–555.89	–146.32	–97.527	–2457.3	–2111.5	

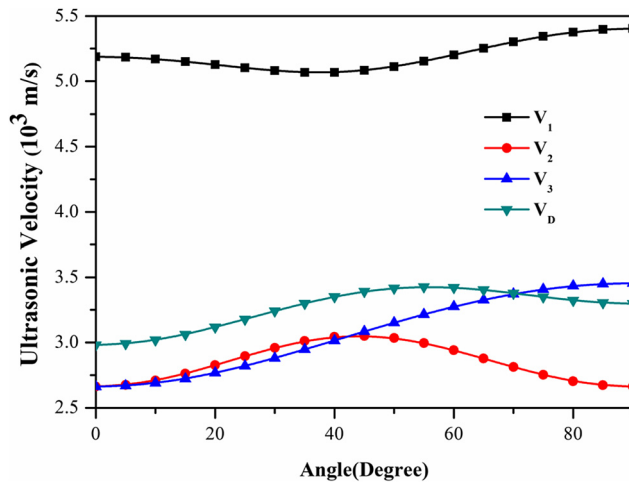


Figure 2: Angle dependent ultrasonic velocities.

It is depicted from Figure 2 that the minimum longitudinal and maximum quasi shear velocities values have been found at 40° and the maximum value of Debye average velocity is at an angle 50° . As we know that Debye average velocity has been obtained by combined values of V_1 , V_2 and V_3 . Although, no direct data is available to compare the velocities of Zr-NW, but the trend of the graph (Figure 2) has been found like other HCP structured materials [14, 15]. The longitudinal ultrasonic velocity (V_L), shear ultrasonic velocity (V_S) and Debye average velocity (V_D) have been evaluated with the help of SOECs and density (ρ) of the Zr-NW. The other thermophysical properties such as specific heat per unit volume (C_v), energy density (E_0) of chosen material have been computed from the AIP Handbook [30]. The thermal conductivity (k) has been evaluated using the Morelli and Slack approach [31]. The acoustic coupling constants (D_L and D_S) and thermal relaxation time (τ) of chosen material have been computed with the help of associated parameters [14, 32]. The anharmonic properties of crystalline material have been understood by the knowledge of Grüneisen parameter. It is the measurement of change in vibrational frequency of atoms of crystalline materials with change in its volume.

This parameter is directly proportional to bulk modulus while is inversely proportional to specific heat and density of the material. We have computed the Grüneisen numbers following the procedure used in our previous work [20, 32]. The coefficient of ultrasonic attenuation over frequency square for longitudinal wave $(\alpha/f^2)_L$ and shear wave $(\alpha/f^2)_S$ under the condition $\omega\tau \ll 1$ and attenuation due to thermo-elastic loss $(\alpha/f^2)_{Th}$ in Zr-NW have been also computed at room temperature. All these evaluated values are presented in Table 2.

From Table 2, the value D_S is less than D_L . This implies that the conversion of ultrasonic energy into thermal energy for the longitudinal ultrasonic wave is greater than that of shear ultrasonic wave for chosen nanowire. The ultrasonic attenuation over frequency square for longitudinal wave $(\alpha/f^2)_L$ and shear wave $(\alpha/f^2)_S$ under the condition $\omega\tau \ll 1$ and attenuation due to thermo-elastic loss $(\alpha/f^2)_{Th}$ in Zr-NW have been also computed at room temperature. All these computed values are presented in Table 2.

In the present evaluation of ultrasonic attenuation, it is supposed that the ultrasonic wave is propagating along unique axis $\theta = 0$ of the nanowire. It is obvious from Table 2, the value of ultrasonic attenuation due to thermoelastic relaxation mechanism $(\alpha/f^2)_{Th}$ is negligible in comparison to ultrasonic attenuation due to Akhieser loss $[(\alpha/f^2)_L \text{ and } (\alpha/f^2)_S]$. So phonon-phonon interaction mechanism is dominating factor over the total ultrasonic attenuation in Zr-NW at room temperature. Unfortunately, to the best of our knowledge, no previous experimental or theoretical data regarding the ultrasonic attenuations in Zr-NW have been reported previously to allow direct comparisons. But the order and nature of attenuation is quite similar with recently reported data for HCP structured NWs such as ZnO-NWs [10] BeO-NWs [33] and InP-NWs [34]. The results obtained in the present study together with the known properties of Zr -NWs provide a more detailed understanding for design of various electronic devices, GMR sensors, bio-magnetic and other medical devices.

Table 2: ρ (10^3 kg m^{-3}), ultrasonic velocities (10^3 ms^{-1}), C_v (10^5 J m^{-3}), E_0 ($10^6 \text{ J m}^{-3} \text{ K}^{-1}$), D_L , D_S , k ($\text{W m}^{-1} \text{ K}^{-1}$), τ (ps), average of Grüneisen number for longitudinal wave $\langle(\gamma_i^j)_L\rangle$, average of square of Grüneisen number for longitudinal wave $\langle(\gamma_i^j)^2\rangle_L$ and shear wave $\langle(\gamma_i^j)^2\rangle_S$, and ultrasonic attenuations over frequency square ($10^{-16} \text{ Nps}^2 \text{ m}^{-1}$) of Zr-NW at room temperature.

ρ	V_L	V_S	V_D	C_v	E_0	k	τ	D_L	D_S
7.466	5.18	2.66	2.98	15.28	249.01	24.6	5.08	174.87	54.80
$\langle\gamma_i^j\rangle_L$	$\langle(\gamma_i^j)^2\rangle_L$	$\langle(\gamma_i^j)^2\rangle_S$		$(\alpha/f^2)_L$	$(\alpha/f^2)_S$		$(\alpha/f^2)_{th}$		$(\alpha/f^2)_{Total}$
-1.14	20.23	6.08		32.13	37.17		0.073		69.38

4 Conclusions

Based on the theoretical calculation of this reveals the following inferences;

- The theory based on simple interaction potential model for the calculation of higher order elastic constants is supported for zirconium nanowires.
- The five independent elastic constants should satisfy the well-known Born's stability criteria imply stable hexagonal structure of chosen nanowire.
- The Pugh's ratio (B/G) shows the ductile nature of chosen nanowire.
- The value of Zener anisotropic ratio (Z_A) is less than one (unity), which confirms the anisotropic behaviour of chosen nanowire.
- The conversion of ultrasonic energy into thermal energy is longitudinal wave greater than that of for the shear wave for chosen nanowire.
- The phonon–phonon interaction mechanism predominant over the thermoelastic loss in chosen nanowire.

The obtained results of elastic constants, ultrasonic velocities, thermal relaxation time and ultrasonic attenuation will provide a base for further investigation of various transport properties of Zr-NWs.

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