



Pressure- and orientation-dependent elastic and ultrasonic characterisation of wurtzite boron nitride

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Abstract. The present study discloses the evaluation of second-order elastic constants of wurtzite boron nitride (w-BN) at room temperature and at different pressures using the many-body interaction potential model approach. Orientation- and pressure-dependent ultrasonic velocity, thermal relaxation time and other related thermophysical parameters (Debye temperature, Debye average velocity, specific heat and thermal energy density) are also calculated using the evaluated second-order elastic constants. The orientation-dependent thermal relaxation time of w-BN is predominantly affected by the Debye average velocity and is indirectly governed by second-order elastic constants. Thermal relaxation time of w-BN is found to decrease with pressure. Calculated elastic and ultrasonic properties of w-BN are compared with the properties of other wurtzite structured materials for a complete analysis and characterisation of the material.

Keywords. Semiconductor; elastic constants; thermal relaxation time; ultrasonic velocities.

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1. Introduction

Boron nitride (BN) is a low porosity white solid material. It is easily machined into complex shapes using standard carbide tooling. The material is anisotropic in its electrical and mechanical properties due to the platy-hexagonal crystals and their orientation during hot press consolidation. BN can stably exist in many polymorphs because B and N atoms can bind together by sp^2 and sp^3 hybridisations. BN can be found in hexagonal/layered graphite-like phase (h-BN, r-BN), turbostratic-like phase (t-BN), cubic diamond-like phase (c-BN) and wurtzite-like phase (w-BN) [1,2]. BN is normally found in hexagonal phase. Hexagonal BN (h-BN) is a stable phase under ambient conditions. Cubic BN and wurtzite BN are synthesised from h-BN at high temperature and high pressure [1–3].

The wurtzite (Wz) phase of BN is in the metastable phase in nature. This material attracts keen interest due to its technological features such as extreme hardness, high melting point, interesting dielectric and thermal behaviour. The structural, mechanical and electronic properties and the stability of BN in $Pnma$ structure were studied using the first-principles calculations by Cambridge Serial Total Energy Package (CASTEP)

plane-wave code, and the calculations were performed with the local density approximation [4]. The thermal conductivity of BN and its composites is reported elsewhere [1,2,5,6]. For thermal management applications, BN is found to be an electrically insulating counterpart of graphene [7,8]. The insulating behaviour of this material along with its high thermal conductivity generates a new concept for the electronic industry.

Wurtzite phase of BN belongs to III group nitrides (GaN, AlN, InN) [9–14]. The structural, elastic, mechanical and acoustical properties of different phases of BN measured using X-ray diffraction, pseudo-potential, DFT methods have been reported in [1,2,9–14]. Very few studies have been done in the past on the pressure-dependent elastic, structural and physical properties of boron compounds [15–17]. Therefore, the present study concentrates on the elastic and ultrasonic characterisation of w-BN under the effect of pressure.

Theoretical evaluation of the second-order elastic constants of w-BN has been done at room temperature and at different pressures using the many-body interaction potential model approach. Orientation- and pressure-dependent ultrasonic velocity, thermal relaxation time and other related thermophysical parameters (Debye temperature, Debye average velocity, specific

heat and thermal energy density) are also calculated using the evaluated second-order elastic constants. The obtained results are compared with the properties of other Wz structured materials for complete analysis and characterisation.

2. Theory

2.1 Theory of elastic constants

The hexagonal structured crystals are mainly classified as close-packed (hcp) and Wz structures. It has long been recognised that the crystals having Wz and sphalerite (zinc blende or ZB) structures are fundamentally similar despite the differences between the two structures [18]. ZB crystals are fcc (Td) with two atoms per primitive cell, whereas Wz crystals are hexagonal (C_{6v}) with four atoms per cell. The fundamental relation between the two structures is that the local environment of any atom in either ZB or ideal Wz ($c/a = 1.633$) is exactly the same through the second neighbour [18]. The maximum packing fraction of the hexagonal structured crystals is similar to fcc. The fraction of the total volume occupied by the atoms is 0.74 for both structures [19]. The formulation for calculating the second-order elastic constants of hexagonal structured crystals are performed using many-body interaction up to second nearest neighbour between the atoms. The formulation is basically done by taking the hexagonal close-packed structured crystal.

The elastic constant of n th order is defined as [20]

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

where F is the free energy density of the material and η_{ij} is the Lagrangian strain component tensor. The total free energy density F can be expanded in terms of strain η using the Taylor series expansion as [21,22]

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

Hence, the free energy density as a function of the square term of strain is written as

$$F_2 = \frac{1}{2!} C_{ijkl} \eta_{ij} \eta_{kl}. \quad (3)$$

For the hexagonal structured material, the basis vectors are $a_1 = a(\sqrt{3}/2, 1/2, 0)$, $a_2 = a(0, 1, 0)$ and $a_3 = (0, 0, c)$ in Cartesian system of axes.

Here a and c are the unit cell parameters. Unit cell of the hexagonal material consists of two non-equivalent atoms: six atoms in the basal plane and three–three atoms above and below the basal plane. Thus, both the first and second neighbourhood consists of six atoms each. $r(1) = a(0, 0, 0)$ and $r(2) = (a/2\sqrt{3}, a/2, c/2)$ are the position vectors of these two types of atoms.

The potential energy per unit cell up to the second neighbourhood is written as

$$U_2 = \sum_{I=1}^6 U_r(I) + \sum_{J=1}^6 U_r(J). \quad (4)$$

Here I is the atom in the basal plane and J is the atom above and below the basal plane. When the crystal is deformed homogeneously, the interatomic vectors in an undeformed state (r) and deformed state (r') are related as

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

where ε_i and ε_j are the Cartesian components of the vector r . The energy density U_r can be expanded in terms of ρ [21,22],

$$U_r = (2V_C)^{-1} \sum \frac{1}{n!} \rho^n D^n \phi(r). \quad (6)$$

Therefore, eq. (4) can be written as

$$U_2 = (2V_C)^{-1} \left[\sum_{I=1}^6 \frac{1}{2!} \rho^2(I) D^2 \phi r(I) + \sum_{J=1}^6 \frac{1}{2!} \rho^2(J) D^2 \phi r(J) \right], \quad (7)$$

where $V_C = 3\sqrt{3}a^2c/2$ is the volume of the elementary cell and $D = R^{-1}(d/dR)$. $\phi(r)$ is the interaction potential and is given by

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

where a_0 and b_0 are constants. Comparing eqs (3) and (7), the crystal symmetry leads to six second-order elastic constants, which are written as

$$\left. \begin{aligned} C_{11} &= 24.1p^4C', & C_{12} &= 5.918p^4C', \\ C_{13} &= 1.925p^6C', & C_{33} &= 3.464p^8C', \\ C_{44} &= 2.309p^4C', & C_{66} &= 9.851p^4C', \end{aligned} \right\} \quad (9)$$

where $p = c/a$, the axial ratio, $C' = \chi a/p^5$, χ is the harmonic parameter. The rest of the second-order elastic constants have a zero value because under 180° rotation they have equal and opposite value for the same stress. The potential energy can be expanded in terms of difference in squares of interatomic distances of deformed

and undeformed states of the crystal. The expansion up to square term can be written as

$$\varphi = \varphi_0 + \chi \sum_{i=1}^2 [\Delta r_i^2]^2. \quad (10)$$

According to eq. (10), χ can be defined as

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

On solving eq. (11) for hexagonal closed-packed structured materials, we have

$$\chi = (1/8)[\{nb_0(n - m)\}/\{a^{n+4}\}]. \quad (12)$$

The parameter χ can be calculated using eq. (12) with appropriate values of a , m , n and b_0 . The lattice parameters (a , c) of w-BN are functions of pressure [15,16]:

$$\frac{a}{a_0} = 1.000 - 9.230 \times 10^{-4} P + 5.580 \times 10^{-6} P^2 - 3.817 \times 10^{-8} P^3, \quad (13)$$

$$\frac{c}{c_0} = 1.000 - 9.076 \times 10^{-4} P + 5.689 \times 10^{-6} P^2 - 4.140 \times 10^{-8} P^3. \quad (14)$$

Here a_0 and c_0 are lattice parameters at zero pressure. Thus, the pressure-dependent second-order elastic constant can be determined using pressure-dependent lattice parameters. The bulk modulus (B) of Wz structured material can be determined by the following expression using the second-order elastic constants:

$$B_0 = \frac{(C_{11} + C_{12}) C_{33} - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}}. \quad (15)$$

2.2 Theory of ultrasonic velocity

There are three types of acoustical wave velocity in hexagonal structured crystals: one longitudinal and two shear wave velocities that are well related to the second-order elastic constants. The velocities can be given by the following expressions [23]:

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

$$V_2^2 = \left\{ \begin{aligned} &C_{33} \cos^2 \theta + C_{11} \sin^2 \theta + C_{44} \\ &- \{[C_{11} \sin^2 \theta - C_{33} \cos^2 \theta + C_{44}(\cos^2 \theta - \sin^2 \theta)]^2 \\ &+ 4 \cos^2 \theta \sin^2 \theta (C_{13} + C_{44})^2\}^{1/2} / 2d \end{aligned} \right\}, \quad (17)$$

$$V_3^2 = \{C_{44} \cos^2 \theta + C_{66} \sin^2 \theta\} / d. \quad (18)$$

In the above equations, V_1 , V_2 and V_3 are velocities of the longitudinal wave, quasishear wave and shear wave, respectively. d and θ are density of the material and angle with the unique axis (z -axis) of the crystal. Density of the Wz structured material can be determined by the following expression [24]:

$$d = \frac{2Mn}{3\sqrt{3} a^2 c N_A}, \quad (19)$$

where M , N_A and n are the molecular weight, Avagadro number and number of atoms per unit cell, respectively.

Debye average velocity is an important parameter in low-temperature physics because it is related to elastic constants through ultrasonic velocities. Debye average velocity (V_D) for wave propagation at any angle with the unique axis is defined as [23]

$$V_D = \left[\frac{1}{3} \left(\frac{1}{V_1^3} + \frac{1}{V_2^3} + \frac{1}{V_3^3} \right) \right]^{-1/3}. \quad (20)$$

If elastic constants are known, the theoretical evaluation of ultrasonic velocity can be done. The Debye temperature (T_D) is indirectly related to elastic constants through the Debye average velocity [23]

$$T_D = \frac{\hbar V_D (6\pi^2 n_a)^{1/3}}{K_B}. \quad (21)$$

Here, \hbar is the quantum of action and is equal to Planck's constant divided by 2π , K_B is the Boltzmann constant and n_a is the atom concentration. On the propagation of the ultrasonic wave, the thermal distribution of phonon is disturbed. The time taken for the re-establishment of equilibrium of the thermal phonons is called the thermal relaxation time (τ) and is given by the following equation:

$$\tau = 3k / C_V V_D^2. \quad (22)$$

Here τ is the thermal relaxation time, k and C_V are the thermal conductivity and specific heat per unit volume of the material, respectively. The specific heat per unit volume is a function of T_D/T and can be determined using literatures [19,25].

Table 1. Parameters of w-BN at different pressure and at room temperature.

Pressure → Parameters ↓		0 GPa	10 GPa	20 GPa	30 GPa	40 GPa	50 GPa	60 GPa
a (Å)	Present	2.55	2.53	2.51	2.49	2.48	2.47	2.46
	[15]	2.548	2.529	2.504		2.479		2.452
	[16]	2.554	2.532	2.512	2.493	2.476		
c (Å)	Present	4.20	4.18	4.15	4.12	4.10	4.08	4.06
	[15]	4.214	4.182	4.143		4.107		4.074
	[16]	4.224	4.188	4.156	4.126	4.098		
ρ (10^3 kg/m ³)		3.512	3.585	3.668	3.755	3.803	3.853	3.904
C_{11} (GPa)		816.1	880.3	952.4	1031.1	1074.1	1119.8	1166.8
C_{12} (GPa)		200.4	216.2	233.9	253.2	263.8	275	286.5
C_{13} (GPa)		176.8	191.9	207.9	225.2	234.4	243.8	253.7
C_{33} (GPa)		863.1	942.4	1022.1	1109.2	1152.7	1195.8	1243.1
C_{44} (GPa)		212.1	230.2	249.3	270.3	281.2	292.4	304.4
C_{66} (GPa)		320	345.2	373.5	404.4	421.2	439.1	457.6
B (GPa)		400.3	433.5	469.4	508.6	529.4	551	573.7
T_D (K)		1436.5	1491.7	1546.5	1604.1	1632.6	1661.1	1691.0
C_V (10^6 J/m ³ K)		1.392	1.323	1.287	1.236	1.207	1.184	1.16
E_0 (10^8 J/m ³)		1.385	1.266	1.176	1.147	1.117	1.089	1.058

3. Results

Initially, the pressure-dependent lattice parameters of w-BN at 300 K are determined using eqs (13) and (14) and zero pressure lattice parameters [1,13,14]. The values of m and n for w-BN are taken as 6 and 7, respectively. Lennard-Jones constant b_0 for w-BN is determined under equilibrium condition and is 7.44×10^{-65} erg cm⁷. Pressure-dependent second-order elastic constants are calculated using pressure-dependent lattice parameters, m , n , b_0 and eq. (9). Pressure-dependent bulk modulus is evaluated with the help of eq. (15) using second-order elastic constants. Pressure-dependent lattice parameters, second-order elastic constants and bulk modulus are given in table 1. Pressure-dependent densities of w-BN are calculated with eq. (19) and are given in table 1.

Ultrasonic velocities are evaluated using eqs (16)–(18) with the help of second-order elastic constants and densities for ultrasonic wave propagation at a different orientation from the unique axis of the w-BN crystal. Debye average velocity at different pressure and orientation from the unique axis is calculated using eq. (20). Ultrasonic velocities V_1 , V_2 , V_3 and V_D are shown in figures 1–4. Debye temperature of w-BN is calculated with the help of eq. (21) at different pressure and at 300 K, which is shown in table 1. The specific heat at constant volume (C_V) and energy density (E_0) are obtained using Debye temperature and [24]. The values of C_V and E_0 are given in table 1 and figure 5. Thermal conductivity of w-BN is reported elsewhere [1]. Thermal relaxation time is determined with the help of eq. (22)

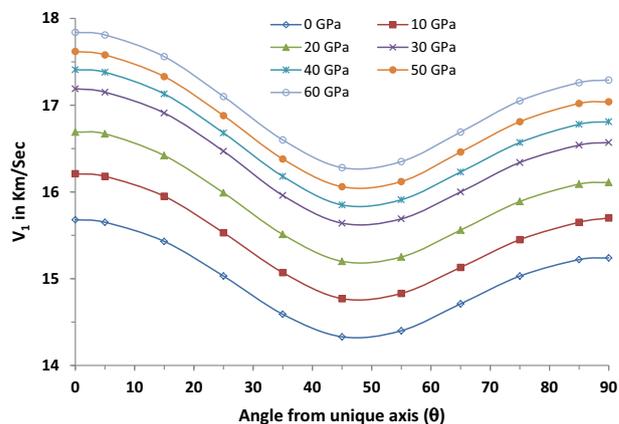


Figure 1. Longitudinal wave velocity vs. angle from the unique axis of the BN crystal.

using k , C_V and V_D at zero external pressure and at temperature 300 K for wave propagation along the unique axis of w-BN crystal. Pressure-dependent V_D and τ are plotted in figure 6.

4. Discussion

A perusal of table 1 indicates that lattice parameters the w-BN decrease with pressure and are in good agreement with the experimental [15] and theoretical [16] values reported in the literature. Table 1 also reveals that the calculated second-order elastic constants and bulk modulus increase with pressure. Due to external pressure, the lattice parameter of w-BN

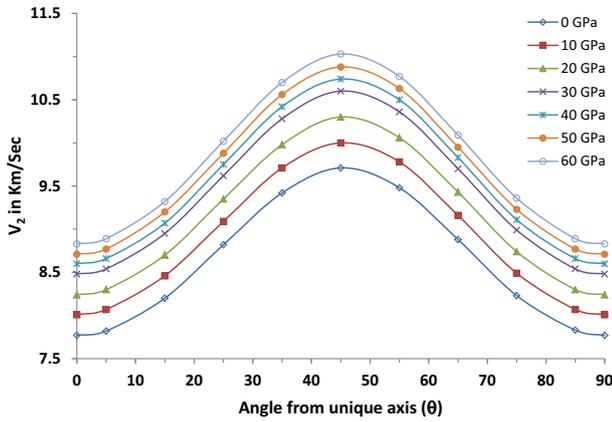


Figure 2. Quasishear wave velocity vs. angle from the unique axis of the BN crystal.

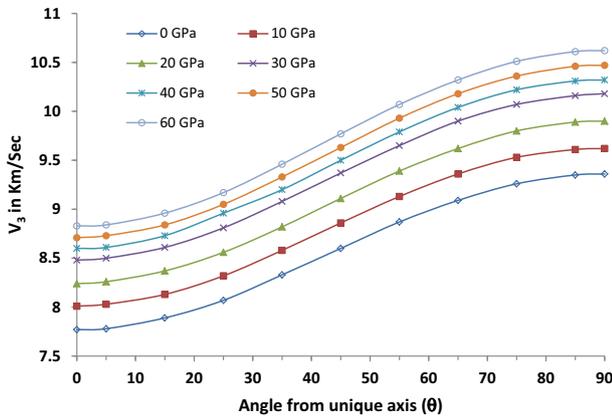


Figure 3. Shear wave velocity vs. angle from the unique axis of the BN crystal.

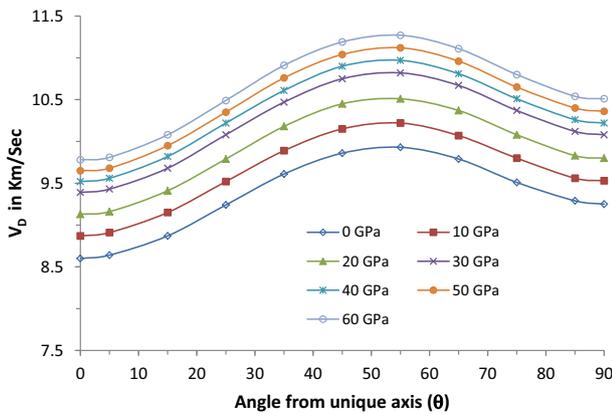


Figure 4. Debye average velocity vs. angle from the unique axis of the BN crystal.

crystal reduces. This causes a reduction in interatomic distance. Therefore, the interatomic force increases with the applied external pressure which results in the enhancement of stress-bearing capacity of a material. Therefore, the increase in elastic constant values is

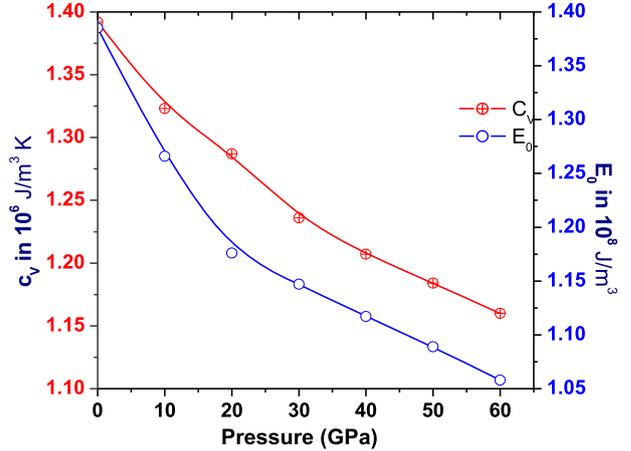


Figure 5. C_V and E_0 vs. pressure for w-BN.

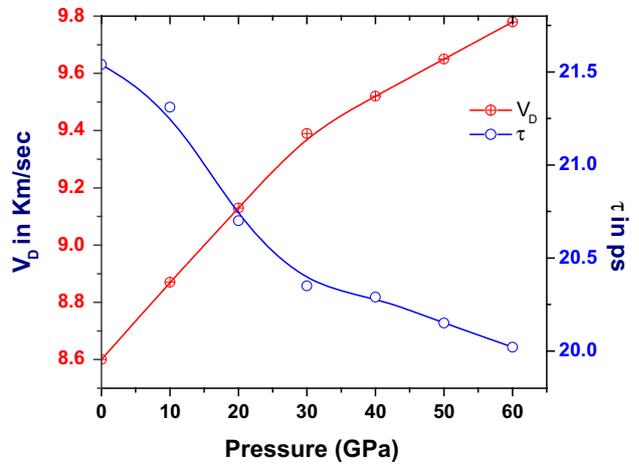


Figure 6. V_D and τ vs. pressure for w-BN.

obtained with the increase in pressure. The reported values of second-order elastic constants C_{11} , C_{33} , C_{44} , C_{66} and bulk modulus of w-BN at room temperature are 982/987, 1077/1020, 388/369, 424/422 and 400/395 GPa, respectively [13,14]. At zero external pressure and 300 K, bulk modulus is exactly the same as the reported value. Second-order elastic constants at 30 GPa are very close to their corresponding reported values. Hence, our evaluated second-order elastic constants of w-BN at a different pressure under potential model approach are justified. Since our potential model approach for the evaluation of second-order elastic constants needs only lattice parameter initially and provides good results and avoids approximations as required in the first principle calculations, it is better than the other model. The density of the hexagonal Wz structured material is inversely proportional to a^2c [24] and the lattice parameters of the selected material are reported to decrease with pressure [15]. Hence, the calculated density of w-BN at different pressure is found to increase

with pressure (table 1). The elastic constants of w-BN are found to be too large in comparison with the nitrides from the same group (AlN, GaN, InN) [26]. Therefore, its mechanical behaviour will be better than the same group nitrides and improves under external pressure. Mechanical strength, hardness and durability of the material are related to their anisotropic elastic constants, and so second-order elastic constants of w-BN are important in manufacturing industries.

The density of w-BN at 300 K is 3.512 g/cm^3 and the density given in the literature is 3.487 g/cm^3 [1,2]. Therefore, our method is justified for calculating pressure-dependent density. On the basis of mode of propagation, there are four types of ultrasonic wave velocities: longitudinal, shear, surface and lamb. Longitudinal and shear wave velocities are more important for the material's characterisation because they are well related to elastic constants and density. Elastic constants of the material are related to the fundamental solid-state phenomenon such as specific heat, Debye temperature and Grüneisen parameters. Elastic constants are related to interatomic forces, coordination changes, etc. and also to the fracture, porosity, crystal growth and microstructural factors (grain shape, grain boundaries, texture, precipitates, etc.). Thus, mechanical behaviour and anisotropic properties of the material under different physical conditions (temperature, pressure, concentration, composition, size, etc.) can be well defined on knowing ultrasonic velocity.

Pressure-dependent ultrasonic velocities (V_1 , V_2 , V_3) and Debye average velocity (V_D) of w-BN crystal at different orientations (figures 1–3) reveal that all the ultrasonic velocities increase with pressure while their nature with orientation resembles the same characteristics as that of the same group of nitrides [26]. The longitudinal ultrasonic velocity (V_1) is minimum along $\theta = 45^\circ$ for w-BN material and quasishear wave velocity (V_2) is maximum along $\theta = 45^\circ$ while pure shear wave velocity (V_3) increases with the direction of orientation with the unique axis. The ultrasonic velocity is directly proportional to the square root of elastic constant and inversely proportional to the square root of density. Yet, both the second-order elastic constants and density of w-BN are found to increase with pressure but the elastic constants play a dominating role towards the enhancement of ultrasonic velocity with pressure. As the elastic constants of w-BN are found to be very high in comparison to elastic constants of the nitrides of the same group (AlN, GaN, InN), the ultrasonic velocities of w-BN have the largest value among IIIrd group nitrides. The present value of V_1 and V_2 or V_3 for wave propagation along the [001] direction ($\theta = 0^\circ$) at 30 GPa is 17.2 and 8.5 km/s, respectively, while velocity for the same direction of propagation are reported to be 17.6

and 10.5 km/s [13]. The good resemblance between the reported and present value of velocities authenticate our evaluated data of ultrasonic velocities.

For determining the specific heat of the material, the essential parameter is the Debye temperature which is directly correlated with the Debye average velocity [19,25]. Pressure-dependent Debye temperature of the w-BN is found to increase with pressure (table 1), as the Debye temperature is indirectly related to elastic constants through the Debye average velocity. The reported Debye temperature at 300 K is 1400 K [1,15] while the present value is 1436.5 K. The first principles calculation reports that the Debye temperature of w-BN increases with pressure and it changes by 15.14% under the application of 40 GPa pressure [16]. In the present evaluation, it is found that the Debye temperature is increased by 13.64% under 40 GPa pressure. Similarity between the present and the reported Debye temperature reveals the justification for the present T_D . Figure 5 indicates that the specific heat and thermal energy density of w-BN decrease as pressure increases. Similar characteristic of w-BN has been reported for C_V [16]. Under pressure, the atoms of the crystal come closer due to a reduction in the basic lattice parameter. Therefore, the loss of heat energy increases by the collision of the surrounding atoms. This causes an increase in loss of heat energy through emission which results in the reduction of C_V with pressure at constant temperature.

It is obvious from figure 6 that the thermal relaxation time of w-BN decreases with pressure at constant temperature. The thermal relaxation time is well correlated with thermal conductivity, Debye average velocity and specific heat of the material. Since thermal conductivity is considered to be constant as it is a function of temperature and the growth rate of V_D is found to be larger than decay rate of C_V thus τ decreases with applied pressure for the w-BN. When the ultrasonic wave propagates through crystalline media, there is an interaction of phonons of the ultrasonic wave and crystal lattice vibrations. Due to this, the thermal energy distribution of thermal phonons is disturbed. The re-establishment time of thermal phonons is termed as thermal relaxation time. The transfer of momentum among atoms becomes fast as pressure increases due to a reduction in atomic separation. Therefore, the re-establishment time for thermal phonons reduces with pressure at constant temperature. The phonon–phonon interaction is one of the major causes for ultrasonic attenuation in the pure crystalline medium [23]. Therefore, it can be predicted that ultrasonic attenuation due to phonon–phonon interaction in w-BN will decrease with pressure. Quantity τ for w-BN is of the order of picosecond, which is the same as that reported for

the same group nitrides in the literature [26]. Thermal relaxation time of w-BN is 21.5 ps at zero pressure and at 300 K. The reported values of τ for GaN, AlN and InN are 32.5, 16.5 and 47.2 ps, respectively. Hence, it can be said that ultrasonic attenuation due to phonon–phonon interaction in w-BN will lie between the ultrasonic attenuations of GaN and AlN.

5. Conclusion

On the basis of the above discussion, we conclude that our potential model theory for the evaluation of second-order elastic constants is justified for w-BN. Density, elastic constant, ultrasonic velocity and Debye temperature of w-BN were found to increase with pressure at constant temperature while specific heat, thermal energy density and thermal relaxation time were found to decrease with pressure at constant temperature. This study on the change in properties of w-BN with pressure will open up new avenues for further investigation and application of this material.

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