VNU Journal of Science: Mathematics – Physics, Vol. 32, No. 2 (2016) 43-53

Mechanical and Thermophysical Properties of Neptunium Monopnictides

Devraj Singh[1,*], Shivani Kaushik[2], Sunil Kumar Pandey[2],
Giridhar Mishra[1], Vyoma Bhalla[1,3]

[1] *Department of Applied Physics, Amity School of Engineering and Technology, New Delhi-110061, India*
[2] *Department of Physics, NIMS University, Jaipur-303121, India*
[3] *Amity Institute of Applied Sciences, Amity University Uttar-Pradesh, Noida-201313, India*

Received 14 April 2016
Revised 25 April 2016; Accepted 20 June 2016

Abstract: The temperature dependent ultrasonic parameters like ultrasonic attenuation, acoustic coupling constant, ultrasonic Grüneisen parameter and ultrasonic velocity at room temperature have been computed for neptunium monopnictides (NpX, where X=N, P, As, Sb). For the evaluation of ultrasonic parameters, the higher order elastic constants have been found out using Coulomb and Born-Mayer potential up to second nearest neighbour in the temperature range 0-300K. In addition to this, some mechanical constants like bulk modulus, Young's modulus and Poisson's ratio are also evaluated at room temperature to find their mechanical stability. The toughness to fracture ratio is found to be 0.571 which clearly shows brittle nature of NpX. Born criterion of mechanical stability is also followed by these materials. Neptunium nitride is most stable and durable material due to its high valued elastic constants. In present investigation, the thermal conductivity of these materials is also evaluated using Slack's approach. The ultrasonic attenuation due to thermoelastic relaxation mechanism is negligible in comparison to phonon-phonon interaction mechanism. The achieved investigation results on NpX materials are discussed and compared with other similar type of materials.

Keywords: Monopnictides, Elastic properties, Ultrasonic properties, Thermal conductivity.

1. Introduction

The studies on rare-earth monochalcogenides and monopnictides have been found extensively in literature [1-5]. The main characteristic of these materials is their partially filled f-orbital which leads to their anomalous behaviour [6-8]. The magnetic properties of neptunium monochalcogenides have been studied by Troc [9]. Jha et al. [10] investigated structural phase transitions and elastic properties of neptunium compounds at high pressure. Braithwaite et al. [11] analysed the pressure effects of magnetism in uranium and neptunium monopnictides. Wachter et al. [12] made analysis of the

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[*] Corresponding author. Tel.: +91-11-2806-2105
Email: dsingh13@amity.edu

electronic and elastic properties of light actinide telluride. The ultrasonic study of neptunium monochalcogenides was carried out by Singh et al. [13]. Trinath et al. [14] studied the structural transitions of neptunium arsenide induced by pressure. The magnetic phase diagram with resonant X-ray magnetic scattering on a single crystal of NpP have been studied by Longfield et al. [15]. The structure of neptunium monopnictides was explained by Vogt and Mattenberger [16]. Nakajima et al. [7] and Sanchez et al. [9] also discussed about the structure of neptunium monopnictides.

To the best of our knowledge, there is no evidence of ultrasonic study of neptunium monopnictides in literature. This stimulated us to study the ultrasonic and mechanical properties of neptunium monopnictides. This work provides the theoretical computation of ultrasonic velocities for longitudinal and shear modes of propagation, Debye average velocity, Debye temperature, thermal conductivity, Breazeale's nonlinearity parameter, ultrasonic attenuation along <100>, <110> and <111> directions at room temperature. Additionally second and third order elastic constants have been computed in the temperature range 0-300K. The obtained results are discussed in correlation with available findings of similar type of materials.

2. Theoretical Approach

Theoretical approach is categorised in following phases:

2.1. Calculation of Second and Third Order Elastic Constants

The SOEC and TOEC of neptunium monopnictides have been calculated using Coulomb and Born Mayer potential [17] at absolute zero. The interionic potential is the sum of electrostatic/Coulomb and repulsive/Born-Mayer potentials.

$$\varphi(r) = \varphi(C) + \varphi(B) \tag{1}$$

Where $\phi(C)$ is long range electrostatic/Coulomb potential and $\phi(B)$ is the short range repulsive/Born-Mayer potential, given as

$$\varphi(C) = \pm(e^2 / r_0) \text{ and } \varphi(B) = A\exp(-r_0 / b). \tag{2}$$

Here 'e' is electronic charge, r is the nearest neighbour distance, b is the hardness parameter and A is the strength parameter [18].

$$A = -3b\frac{e^2}{r_0^2}S_3^{(1)}\frac{1}{6\exp(-\rho_0)+12\sqrt{2}\exp(-\sqrt{2}r_0)} \tag{3}$$

Where $\rho_0 = \frac{r_0}{b}$.

As per theory given by Leibfried [19], lattice energy changes with temperature, thus by addition of vibrational energy contribution to static elastic constants, we get temperature dependent second and third order elastic constants (C_{IJ} and C_{IJK}) at required temperature.

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{Vib} \quad and \quad C_{IJK} = C_{IJK}^0 + C_{IJK}^{Vib} \tag{4}$$

Hiki [18] and Ghate [20] developed the method of calculating the elastic constants at higher temperature. The detailed expression for higher order elastic constants are given in literature [21].

The density, Poisson's ratio (ν), Zener's anisotropy(A) and tetragonal moduli C_S) are also evaluated using formulae as given below:

The bulk modulus $B_T = \frac{C_{11} + 2C_{12}}{3}$ (5)

Poisson's ratio, $\nu = \frac{3B_T - 2G}{6B_T + 2G}$ (6)

Shear modulus, $G = \frac{G_V + G_R}{2}$ (7)

Where $G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}$ (8)

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \qquad (9)$$

Tetragonal moduli, $C_S = \frac{C_{11} - C_{12}}{2}$ (10)

The distortion produced due to the propagation of ultrasonic waves characterise the simple harmonic generation of longitudinal waves given by negative ratio of nonlinearity term to the linear term in non linear waves [21-22] given by:

$\beta = -(3K_2+K_3)/K_2$ (11)

K_2 and K_3 are linear combinations of SOEC and TOEC respectively. The expressions for K_2 and K_3 are shown below:

Direction	K_2	K_3
<100>	C_{11}	C_{111}
<110>	$\frac{C_{11} + C_{12} + 2C_{44}}{2}$	$\frac{C_{111} + 3C_{112} + 12C_{166}}{4}$
<111>	$\frac{C_{11} + 2C_{12} + 4C_{44}}{3}$	$\frac{C_{111} + 6C_{112} + 12C_{144} + 24C_{166} + 2C_{123} + 16C_{456}}{9}$

2.2. Calculation of Ultrasonic Velocities and Debye Temperature

The ultrasonic velocities along <100>, <111>, <110> directions are calculated for longitudinal and shear modes of propagation. The expressions for longitudinal and shear velocities along different directions and Debye average velocity are given in literature [21]. The expressions for Debye temperature as given in literature [21] is given as:

$$\theta_D = \frac{h}{k_B}\left(\frac{3n}{4\pi}\frac{N\rho}{M}\right)^{\frac{1}{3}} V_D \qquad (12)$$

Where h is Planck's constant, k_B the Boltzmann constant, N the Avogadro's number, ρ the density, M the molecular weight, n the number of atoms in the molecule, V_D the mean sound velocity (or Debye average velocity) . For an isotropic crystals V_D is given by:

$$V_D = \left(\frac{1}{3}\left(\frac{1}{V_L^3} + \frac{2}{V_S^3}\right)\right)^{-\frac{1}{3}} \qquad (13)$$

V_L and V_S are longitudinal and shear velocities respectively.

2.3. Evaluation of Thermal Conductivity

Heat can be transferred in a material both by charge carriers and vibrations of lattice ions. In materials where there are no free charge carriers, heat is conducted through lattice vibrations. Thermal conductivity here means heat conduction through vibrations of lattice ions in a solid. Thermal phonons responsible for carrying heat undergo scattering events proportional to the number of scattering sites present including defects. The standard treatment of thermal conductivity of solids is based on Debye's extension of kinetic theory of gases. There are two methods for finding the thermal conductivity. One considers the phonon relaxation time and the other considers the phonon mean free path. Callaway and Baeyer [24] calculated the thermal conductivity by considering the relaxation time method. Roufosse and Klemens [25] calculated the thermal conductivity on the basis of changing mean free path. The phonon frequency is directly proportional to temperature. Klemens [26] reviewed the influence of various type of defects on lattice thermal conductivity. Slack [27] and Berman [28] derived the expression to find out the thermal conductivity at room temperature near the Debye temperature of solids. The expression for finding thermal conductivity in solid materials is

$$\kappa = \frac{A\overline{M}_a \theta_D^3 \delta n^{\frac{1}{3}}}{\gamma^2 T} \tag{14}$$

where A is a constant having value $3.04\text{x}10^{-8}$, M_a is the atomic mass of atom (in amu), $\overline{M}_a$ is the average atomic mass given by $M_a/2$, δ in is the volume per atom [29], n is the number of atoms per unit cell and γ is the Grüneisen parameter.

2.4. Ultrasonic Attenuation

At higher temperature, ultrasonic attenuation is mainly caused by thermoelastic phenomenon as well as phonon-phonon interaction process [25].

The total ultrasonic attenuation is summation of loss due to thermoelastic relaxation and phonon-phonon interaction mechanisms i.e.,

$$\left(\frac{\alpha}{f^2}\right)_{Total} = \left(\frac{\alpha}{f^2}\right)_{Th} + \left(\frac{\alpha}{f^2}\right)_{Akh} \tag{15}$$

Where α =ultrasonic absorption coefficient

f= frequency of ultrasonic wave

Th refers thermoelastic loss and Akh refers phonon-phonon interaction for longitudinal and shear modes in Akhieser regime.

The ultrasonic absorption coefficient over frequency square due to thermoelastic relaxation mechanism is obtained by following expression:

$$\left(\frac{\alpha}{f^2}\right)_{Th} = \frac{4\pi^2 < \gamma_i^j >^2 \kappa T}{2\rho V_L^5} \tag{16}$$

Where γ_i^j = Gruneisen parameter, κ = thermal conductivity of the material, ρ = density of the material and V_L = ultrasonic velocity for longitudinal wave

The ultrasonic absorption coefficient over frequency square due to phonon- phonon interaction (Akhieser loss) is expressed as:

$$\left(\frac{\alpha}{f^2}\right)_{long} = \frac{4\pi^2 \tau E_0 \frac{D_L}{3}}{2\rho V_L^3} \tag{17}$$

$$\left(\frac{\alpha}{f^2}\right)_{shear} = \frac{4\pi^2 \tau E_0 \frac{D_S}{3}}{2\rho V_S^3} \tag{18}$$

Where E_0 = energy density of the material

V_S = ultrasonic velocity for shear wave

τ is the thermal relaxation time.

Table 1. Computed values for SOEC and TOEC for neptunium monopnictides (with comparison with other materials) in the order 10^{10}N/m^2

Material	Temp	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
NpN	0K	6.42	2.76	2.76	-98.57	-11.3	4.35	4.35	-11.3	4.35
	100K	6.79	2.67	2.78	-101.03	-11.01	3.91	4.39	-11.39	4.35
		6.84^a	2.49^a	2.60^a	-110.5^a	-10.28^a	3.66^a	4.19^a	-10.7^a	4.16^a
	300K	7.13	2.49	2.79	-102.1	-10.45	3.02	4.45	-11.46	4.35
		7.6^a	2.3^a	2.61^a	-111.6^a	-9.64^a	2.65^a	4.25^a	-10.76^a	4.16^a
		6.2^b	2.09^b	2.29^b	-89.77^b	-8.65^b	2.8^b	3.65^b	-9.44^b	3.59^b
NpP	0K	5.08	1.51	1.51	-84.12	-6.15	2.52	2.52	-6.15	2.52
	100K	5.34	1.43	1.52	-85.75	-5.84	2.04	2.54	-6.19	2.52
		5.3^a	1.36^a	1.45^a	-86.14^a	5.55^a	1.93^a	2.44^a	-5.9^a	2.42^a
		4.35^c	1.02^c	1.09^c	-72.09^c	-4.13^c	1.4^c	1.87^c	-4.44^c	1.85^c
	300K	5.67	1.28	1.53	-87.31	-5.23	1.09	2.58	-6.24	2.52
		5.64^a	1.19^a	1.46^a	-87.73^a	4.92^a	0.95^a	2.47^a	-5.95^a	2.42^a
		4.66^c	0.87^c	1.1^c	-73.56^c	-3.55^c	0.5^c	1.9^c	-4.48^c	1.85^c
NpAs	0K	4.70	1.27	1.27	-79.7	-5.16	2.16	2.16	-5.16	2.16
	100K	4.91	1.19	1.28	-80.99	-4.85	1.67	2.17	-5.19	2.16
		4.96^a	1.2^a	1.28^a	-81.91^a	-4.88^a	1.68^a	2.18^a	-5.22^a	2.17^a
		4.74^c	1.36^c	1.44^c	-75.51^c	-5.59^c	1.95^c	2.39^c	-5.89^c	2.37^c
	300K	5.26	1.03	1.3	-82.75	-4.23	0.07	2.21	-5.23	2.16
		5.31^a	1.04^a	1.29^a	-83.69^a	-4.25^a	0.7^a	2.22^a	-5.27^a	2.17^a
		5.07^c	1.21^c	1.45^c	-77.07^c	-5.05^c	1.17^c	2.43^c	-5.95^c	2.37^c
NpSb	0K	4.07	0.94	0.94	-71.94	-3.78	1.64	1.64	-3.78	1.64
	100K	4.26	0.87	0.95	-73.09	-3.47	1.14	1.65	-3.8	1.64
		4.34^a	0.9^a	0.98^a	-74.15^a	-3.63^a	1.2^a	1.71^a	-3.96^a	0.17^a
	300K	4.59	0.72	0.95	-74.91	-2.84	0.15	1.67	-3.83	1.64
		4.68^a	0.75^a	0.99^a	-75.97^a	-3^a	0.21^a	1.73^a	-4^a	0.17^a
		4.26^b	0.78^b	0.89^b	-69.5^b	-2.93^b	0.89^b	1.54^b	-3.62^b	1.52^b

[a]Ref. No.32, [b]Ref.No. 24, [c]Ref.No. 33

The expression for thermal relaxation time is

$$\tau_{Th} = \tau_{shear} = \frac{\tau_{long}}{2} = \frac{3\,\kappa}{C_V V_D^2} \tag{19}$$

Where C_V = specific heat per unit volume of the chosen material.

D is the acoustic coupling constant, which is measure of acoustic energy conversion into thermal energy under relaxation process. It can be expressed as:

$$D = 9 < \gamma^2 > -3 < \gamma >^2 \frac{C_V T}{E_0} \tag{20}$$

3. Results and Discussion

3.1. Higher order elastic constants

The second and third order elastic constants are calculated in the temperature range from 0 to 300K The elastic constants are calculated using two input parameters- nearest neighbour distance and hardness parameter. The lattice constants [30] for NpN, NpP, NpAs and NpSb are 2.448 Å, 2.807 Å, 2.915 Å, 3.127 Å respectively. The value of hardness parameter [31] is taken as 0.303Å for all the chosen monopnictides. The values of SOEC and TOEC are calculated using Eqs.(1)- (6) for temperature 0K, 100K and 300K and are shown in Table1. It is obvious from the Table 1 that the values of C_{11}, $C_{44,}$ C_{111}, C_{166} and C_{144} increase with temperature while C_{12}, C_{112} and C_{123} decrease with temperature. The values of C_{456} remain constant. Also, we observed that the decrease in the values of elastic constants with increase in molecular weight. A similar behaviour is shown by berkelium monopnictides [32], ytterbium monopnictides [33] and praseodymium monopnictides [22].

According to Born criteria [23,34] stability is expressed as

$$B_T = (C_{11}+2C_{12})/3>0,\ C_S= (C_{11}- C_{12})/2 > 0\ ,\ C_{44}> 0 \tag{21}$$

The value of bulk modulus (B_T), tetragonal modulus (Cs) and shear modulus (C_{44}) are obtained from Eq. (21) and are given in Table 2.

Table 2. Bulk modulus B_T, C_{44}, C_S (10^{10}N/m^2) at 300K

Material	B_T	C_S	C_{44}
NpN	4.04	2.32	2.79
NpP	2.74	2.19	1.53
NpAs	2.44	2.12	1.30
NpSb	2.01	1.94	0.95

Since all the values of B_T, C_S and C_{44} are greater than 1 as shown in Table 2. Hence the Born criterion is fulfilled by the chosen materials. The ratio of bulk modulus to isotropic shear modulus i.e., G/B (toughness to fracture ratio) is greater than 0.571 so the materials are brittle. The calculated values of (toughness to fracture ratio) G/B for NpN, NpP, NpAs and NpSb are 0.64, 0.64, 0.64 and 0.63 respectively at 300K. The nature of bonding forces can be analysed from Poisson's ratio. For central forces, the value of Poisson's ratio should lie in range $0.25<\nu < 0.5$. For the material considered in our study the value of Poisson's ratio does not fall in the range which means that the forces are non central [34]. The value for Poisson's ratio for NpN, NpP, NpAs and NpSb are 0.24, 0.21, 0,23 and 0.23 respectively by our study. The value of Young's modulus is greater for NpN ($6.40\text{x}10^{10}$ N/m^2) and for NpP, NpAs , NpSb are $4.82\text{x}10^{10}$ N/m^2, $3.89\text{x}10^{10}$ N/m^2 and $3.14\text{x}10^{10}$ N/m^2 respectively . Hence NpN is more stiffer than other materials.

3.2. Deviation from Cauchy's Relation

Cousin [35] and Hiki & Granato [36] proposed that Cauchy relation for SOECs and TOECs at 0K are:

$$C^0_{12} = C^0_{44}; C^0_{112} = C^0_{166}; C^0_{123} = C^0_{465} = C^0_{144} \quad (22)$$

The temperature dependence of ratios C_{44}/C_{12} and C_{166}/C_{112} can be seen from Table 1. The deviation of elastic constants in Table 1, suggest that the forces become more ionic with rise in temperature. The Cauchy's relation is followed at 0K but deviates at higher temperature due to vibrational part of energy.

3.3. Ultrasonic Velocity and Breazeale's Non-linearity Parameter

The variation of Breazeale's non linearity parameter with temperature is shown in Fig.1 along different crystallographic directions. It is seen that the highest value of non linearity parameter is along <100> and lowest along <111> direction. Also the values decrease with increase in temperature.

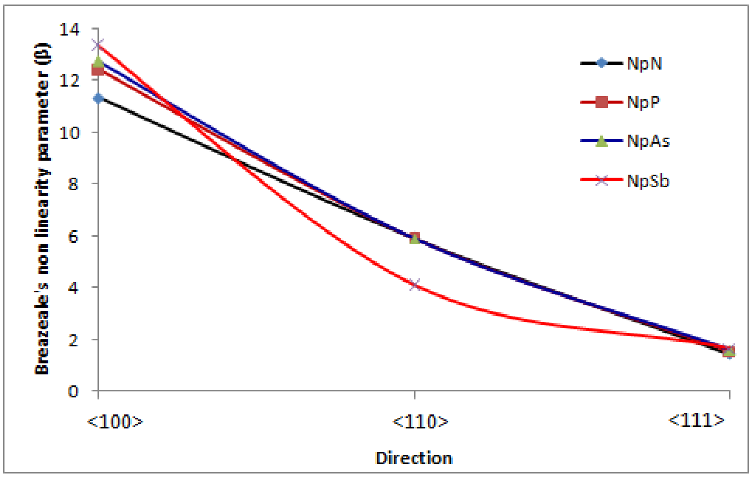

Figure 1. Breazeale's nonlinearity parameter along <100>, <110> and <111> directions at room temperature.

The calculated values of ultrasonic velocity, Debye average velocity along <100>, <110> and <111> directions are shown in Table 3.

Table 3. Ultrasonic velocity of NpX (10^3m/s): V_L for longitudinal waves, V_S for shear waves and Debye average velocity V_D at room temperature along <100>, <110>, <111> directions.

Materials	<100>			<110>				<111>		
	V_L	V_S	V_D	V_L	V_{S1a}	V_{S2b}	V_D	V_L	V_S	V_D
NpN	2.44	1.4	1.54	2.31	1.4	1.81	1.69	2.33	1.32	1.47
NpP	2.37	1.23	1.38	2.22	1.23	2.09	1.59	2.18	1.40	1.54
NpAs	2.25	1.11	1.24	2.06	1.11	2.01	1.46	2.00	1.34	1.46
NpSb	2.17	0.98	1.10	1.93	0.98	1.99	1.31	1.83	1.28	1.39

[a] shear waves polarized along <001> direction

[b] shear waves polarised along $<1\bar{1}0>$ direction

It is seen that the ultrasonic velocities decrease from NpN to NpSb due to increase in molecular weight. The longitudinal wave velocity is maximum along <100> and minimum along <111> direction. The longitudinal wave velocity is maximum for NpP along <100> direction and minimum for NpSb along <111> direction. NpN shows a different behaviour which may be due to the large value of density and C_{11}. The shear wave velocity is maximum along <110> direction polarised along $<1\bar{1}0>$ direction.

The value of Debye average velocity is maximum along <110> and minimum along <111> direction as shown in Table 3. So direction <110> is most suitable for ultrasonic wave propagation. The value of Debye temperature decreases with increase in lattice constant. The value of Debye temperature is maximum along <110> direction except for NpSb which may be due to its low density.

3.4. Thermal Conductivity

The thermal conductivity is calculated using Eq.(14). The variation of thermal conductivity with temperature is as shown in Fig. 2 along different crystallographic directions.

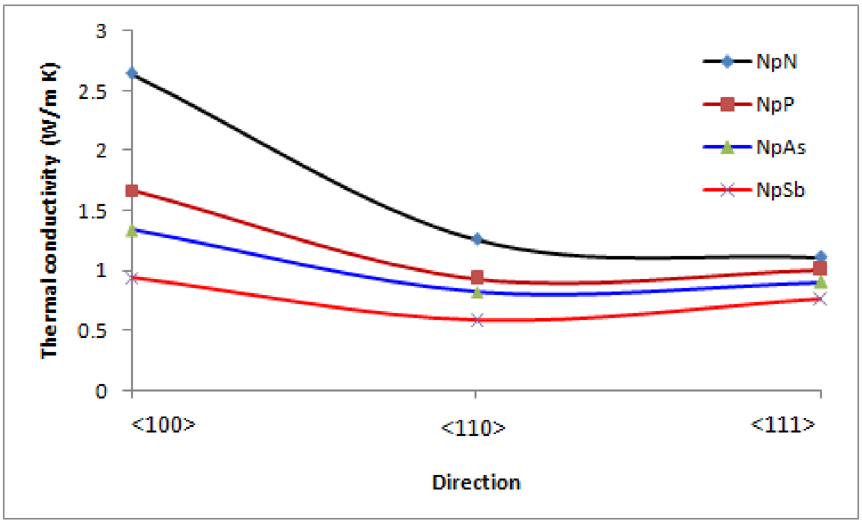

Figure 2. Direction dependent thermal conductivity at room temperature.

Figure 2 shows that there is a decrease in thermal conductivity with increase in temperature and molecular weight. The thermal conductivity is maximum for NpN and minimum for NpSb. Also it is maximum along <100> and minimum along <110> direction.

3.5. Thermal Relaxation Time, Acoustic Coupling Constant and Ultrasonic Attenuation

The thermal relaxation time (τ) and acoustic coupling constants (D) are evaluated by means of Eqs. (19)-(20) respectively. The ultrasonic absorption coefficient over frequency square (α/f^2) due to phonon-phonon interaction and relaxation mechanism is obtained using Eqs. (16)-(18). The obtained values of τ, D and (α/f^2) are given in Table 4. It is obvious from Table 4 that thermal relaxation time increases with increase of molecular weight of NpX. The acoustic coupling constant is a measure of conversion of acoustic energy into thermal energy. The values decrease with increase in temperature. The thermal relaxation time is of the order of picoseconds which confirms semimetallic nature [37,38]. The thermoelastic loss has no significant role in shear wave propagation. It is observed that thermoelastic loss is negligible as compared to Akhieser loss due to lower value of thermal conductivity. The rate of increase or decrease of ultrasonic attenuation depends on energy density and other associated parameters as it affects the phonon-phonon interaction.

Table 4. Thermal relaxation time τ_{th} (ps), acoustic coupling constant (D_l, D_{S1}), ultrasonic attenuation due to thermoelastic loss $(\alpha/f^2)_{th}$ and Akhieser $(\alpha/f^2)_{Akh(l)}$, $(\alpha/f^2)_{Akh(S1)}$ and $(\alpha/f^2)_{Akh(S2)}$ along <100>,<110> and <111> directions at room temperature (all attenuation in $\times 10^{-16}$ Nps^2 m^{-1}).

Material	Direction	τ_{th} (ps)	D_l	D_{S1}	D_{S2}	$(\alpha/f^2)_{th}$	$(\alpha/f^2)_{Akh\ (l)}$	$(\alpha/f^2)_{Akh\ (s1)}$	$(\alpha/f^2)_{Akh\ (s2)}$
NpN	<100>	2.4	12.86	1.08	1.08	0.037	8.5	1.46	1.46
	<110>	0.9	15.69	1.26	21.78	0.042	3.46	0.62	4.99
	<111>	1.1	14.9	14.94	14.94	0.026	4.06	11.19	11.19
NpP	<100>	2.8	14.75	1.08	1.08	0.022	9.5	2.59	2.59
	<110>	1.1	17.28	0.90	26.91	0.049	5.14	0.86	4.79
	<111>	1.3	15.25	18.45	18.45	0.049	5.73	13.08	13.08
NpAs	<100>	3.1	15.49	1.08	1.08	0.023	11.37	3.30	3.30
	<110>	1.4	18.19	0.88	28.62	0.059	7.64	1.20	6.47
	<111>	1.5	15.68	19.53	19.53	0.067	7.71	15.96	15.96
NpSb	<100>	3.4	16.95	1.08	1.08	0.021	13.59	4.70	4.70
	<110>	1.5	19.95	0.81	31.95	0.062	9.8	1.51	7.15
	<111>	1.7	16.47	21.78	21.78	0.098	10.62	20.53	20.53

It is obvious from Table 4 that the order of the thermal relaxation time is of picoseconds, which confirms semimetallic nature of the chosen materials. The variation of total ultrasonic attenuation $[(\alpha/f^2)_{Total} = (\alpha/f^2)_{Th} + (\alpha/f^2)_{Akh}]$ with temperature is shown in Fig. 3. The value of total attenuation is less for NpN along <110> direction. Hence NpN is the best candidate for the industrial applications. The order and nature of ultrasonic attenuation is found similar to other rare-earth materials like lanthanum monopnictides [39], rare-earth monoarsenides [40] and gadolinium monopnictides [41].

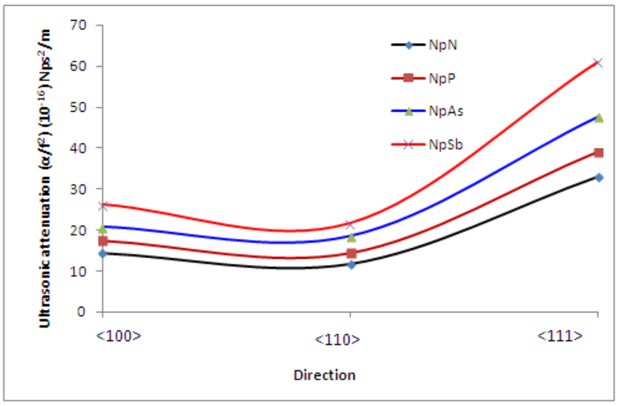

Figure 3. Variation of ultrasonic attenuation along <100>, <110> and <111> directions.

4. Conclusions

Thus, in this study, Born-Mayer model has been applied to find out the higher order elastic constants with the help of two parameters i.e., lattice and hardness constant. The trend of higher order elastic constants i.e., $C_{11}>C_{44}>C_{12}$ and $C_{144}>C_{456}>C_{123}>C_{166}>C_{111}$ is obtained by the proposed theory.

Born-stability criterion has been followed by neptunium monopnictides. Hence they are stable in nature. The ration G/B is found greater than 0.571 in these materials. So these materials have brittle nature. The value of Poisson's ratio does not fall in required range. So we may say that the applied forces are non-central. Cauchy's relations are followed by these materials at 0K, but not at higher temperatures. The Breazeale's non-linearity parameter is highest along <100> direction and lowest along <111> direction at room temperature.

Ultrasonic velocity is found to be highest for NpN along all chosen directions, so NpN will be most suitable material for ultrasonic wave propagation.

The value of thermal relaxation time is of the order of picoseconds, which confirm that the materials have semimetallic nature. The value of thermal conductivity is highest along <100> and lowest along <111> direction. But the nature of ultrasonic attenuation is associated with different thermophysical parameter like thermal relaxation, energy density, specific heat, ultrasonic velocities. The order of ultrasonic attenuation confirmed that the chosen materials are of semimetallic type.

Thus our theoretical approach to calculate the higher order elastic constants, mechanical constants, ultrasonic velocities, thermal conductivity, ultrasonic attenuation is justified and obtained results will be interesting to explore any further physical information of the neptunium monopnictides.

References

[1] G. Vaitheeswaran, L. Petit, A. Svane, V. Kanchana, M. Rajagopalan M, Electronic structure of praseodymium monochalcogenides under pressure, Journal of Physics: Condensed Matter 16 (2004), 4429-4440.

[2] W. Feng, H. Hu, X. Xiao, S. Cui, Z. Lv, G. Zhang, C. Wu, First-principles study of phase transition and elastic properties of XBi (X = Ce, Pr) compounds, Computational Materials Science 53 (2012) 75.

[3] D. Singh, R. Kumar, D.K. Pandey, Temperature and Orientation Dependence of Ultrasonic Parameters in Americium Monopnictides, Advances in Materials Physics and Chemistry 1 (2011) 31.

[4] V. Bhalla, D. Singh, Anisotropic assessment of ultrasonic wave velocity and thermal conductivity in ErX (X:N, As), Indian Journal of Pure & Applied Physics 54 (2016) 40.

[5] I. Shirotani, J. Hayashi, K. Yamanashi, K. Hirano, T. Adachi, N. Ishimatsu, O. Shimomura, T. Kikegawa, X-ray study with synchrotron radiation of cerium and praseodymium monopnictides with the NaCl-type structure at high pressures, Physica B: Condensed Matter 334 (2003) 167.

[6] B. R. Cooper, G. J. Hu, N. Kioussis, J.M. Wills, Theory of anisotropic magnetic behavior in hybridizing actinide systems, Journal of Magnetism and Magnetic Materials 63 (1987) 121.

[7] K. Nakajima, Y. Arai, Y. Suzuki, Vaporization behavior of neptunium mononitride, Journal of Nuclear Materials 247 (1997) 33.

[8] J.P. Sanchez, P. Burlet, S. Quézel, D. Bonnisseau, J. Rossat-Mignod, J.C. Spirlet, J. Rebizant, O. Vogt, Mössbauer spectroscopy and neutron diffraction studies of neptunium antimonide NpSb, Solid State Communications 67 (1988) 999.

[9] R. Troc, Neptunium monochalcogenides: magnetic susceptibility. In Actinide Monochalcogenides, Volume 27B6b of the series Landolt-Börnstein - Group III Condensed Matter, Springer: Berlin Heidelberg, 2009.

[10] P.K. Jha, M. Aynyas, S.P. Sanyal, Structural phase transition and elastic properties of neptunium compounds at high pressure, Indian Journal of Pure and Applied Physics 42 (204) 112.

[11] D. Braithwaite, A. Demuer, I.N. Goncharenko, V. Ichas, J.M. Mignot, J. Rebizant C. Spirlet, O.Vogt, S. Zwirne, Pressure effects on magnetism in the uranium and neptunium monopnictides, Journal of Alloys & Compounds 271 (1998) 426.

[12] P. Wachter, M. Filzmoser, J. Rebizant, Electronic and elastic properties of the light actinide telluride, Physica B: Condensed Matter 293 (2001) 199.

[13] D. Singh, D.K. Pandey, D.K. Singh, R.R. Yadav, Propagation of ultrasonic waves in neptunium monochalcogenides, Applied Acoustics 72 (2011) 737.

[14] C.U.M. Trinath, M. Rajagopalan, S. Natarajan, A computational study of structural transition in NpAs and NpTe induced by pressure, Journal of Alloys & Compounds 274 (1998) 18.

[15] M.J. Longfield, J.A. Paixão, N. Bernhoeft, G.H. Lander, F. Wastin, J. Rebizant, Synchrotron radiation study of neptunium phosphide, Physical Review B 66 (2002) 134421.

[16] O. Vogt, K. Mattenberger, Magnetic measurements on rare earth and actinide monopnictides and monochalcogenides; In: K.A. Gschneidner, L. Eyring, G.H. Lander, G.R. Choppin, Eds., Handbook on the Physics and Chemistry of Rare Earths, Physics-I, Vol. 17, Ch. 1, Lanthanides/Actinides, North-Holland, Amsterdam, 1993.

[17] M. Born, J.E. Mayer, Zur Gittertheorie der Ionenkristalle, Zeitschrift für Physik 75 (1931) 1.

[18] S. Mori, Y. Hiki, Calculation of the third- and fourth-order elastic constants of alkali halide crystals, Journal of the Physical Society of Japan 45 (1975) 1449.

[19] G. Leibfried, H. Hahn, Zur Temperaturabhängigkeit der elastischen Konstanten von Alkalihalogenidkristallen, Zeitschrift für Physik 150 (1958) 497.

[20] P.B. Ghate, Third-order elastic constants of alkali halide crystals, Physical Review 139 (1965) A1666.

[21] V. Bhalla, D. Singh, S.K. Jain, Mechanical and thermophysical properties of cerium monopnictides, International Journal of Thermophysics 37 (2016) 33.

[22] V. Bhalla, R. Kumar, C. Tripathy, D. Singh, Mechanical and thermal properties of praseodymium monopnictides: an ultrasonic study; International Journal of Modern Physics B 27 (2013) 1350116.

[23] W. P. Mason, Effect of impurities and phonon processes on the ultrasonic attenuation of germanium, crystal quartz and silicon; In: Physical Acoustics, IIIB, Chapter 6, Academic Press, New York, 1965.

[24] J. Callaway, H.C. Von Baeyer, Effect of point imperfections on lattice thermal conductivity, Physical Review 120 (1960) 1149.

[25] M.C. Roufosse, P.G. Klemens, Lattice thermal conductivity of materials at high temperatures, Journal of Geophysical Research, 79 (1974) 703.

[26] P.G. Klemens, Thermal conductivity and lattice vibrational modes, Solid State Physics 7 (1958) 1.

[27] G.A. Slack, The thermal conductivity of nonmetallic crystals, Solid State Physics, 34 (1979) 1.

[28] R. Berman, Thermal Conductivity in Solids, Clarendon Press, Oxford, 1976.

[29] C.L. Julian, Theory of Heat Conduction in Rare-Gas Crystals, Physical Review 137, 1965, A128..

[30] A.T. Aldred, B.D. Dunlap, G.H. Lander, Magnetic properties of neptunium Laves phases: high-field measurements on $NpAl_2$ and $NpOs_2$, Physical Review B 14 (1976) 1276.

[31] M.P. Tosi, Cohesion of ionic solids in the Born model; In: Solid State Physics, Vol. 16, Academic Press, New York, 1964..

[32] D. Singh, S. Kaushik, S. Tripathi, V. Bhalla, A.K. Gupta, Temperature dependent elastic and ultrasonic properties of berkelium monopnictides,; Arabian Journal for Science and Engineering 39 (2014) 485.

[33] D.K. Pandey, D. Singh, V. Bhalla, S. Tripathi, R.R. Yadav, Temperature dependence of elastic and ultrasonic properties of ytterbium monopnictides, Indian Journal of Pure & Applied Physics 52 (2014) 330.

[34] J.P. Watt, L. Peselnick, Clarification of the Hashin ‐ Shtrikman bounds on the effective elastic moduli of polycrystals with hexagonal, trigonal, and tetragonal symmetries, Journal of Applied Physics 51 (1980) 1525.

[35] C.S.G. Cousin, New relations between elastic constants of different orders under central force interactions, Journal of Physics C: Solid State Physics, 4 (1971) 1117.

[36] Y. Hiki, A.V. Granato, Anharmonicity in noble metals: higher order elastic constants, Physical Review 144 (1966) 411.

[37] D. Singh, R.R. Yadav, A.K. Tiwari, Ultrasonic attenuation in semiconductors, Indian Journal of Pure & Applied Physics 40 (2002) 845.

[38] D.K. Pandey, D. Singh, R.R.Yadav, Ultrasonic wave propagation in IIIrd group nitrides, Applied Acoustics 68 (2007) 766.

[39] R.R.Yadav, D. Singh, Ultrasonic attenuation in lanthanum monochalcogenides, Journal of the Physical Society of Japan 70 (2001) 1825.

[40] V. Bhalla, D. Singh, S.K. Jain, R. Kumar, Ultrasonic attenuation in rare-earth monoarsenides, Pramana-Journal of Physics, 2016, doi: 10.1007/s12043-015-1183-5.

[41] D. Singh, S. Tripathi, D.K. Pandey, A.K. Gupta, D.K. Singh, J. Kumar, Ultrasonic wave propagation in semimetallic single crystals, Modern Physics Letters B 25 (2011) 2377..