

Temperature and Orientation Dependence of Ultrasonic Parameters in Americium Monopnictides

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Abstract

The temperature dependence of the ultrasonic parameters like ultrasonic velocities and Grüneisen parameters in americium monopnictides AmY (Y: N, P, As, Sb and Bi) have been studied for longitudinal and shear waves along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ crystallographic directions in the temperature range 100 K - 500 K. The second- and third- order elastic constants have also been evaluated for these monopnictides using Coulomb and Born-Mayer potential. The values of elastic constants are the highest for AmN. Hence the mechanical properties of AmN are better than other monopnictides AmP, AmAs, AmSb and AmBi. Ultrasonic velocity is found large for AmP. So the ultrasonic wave propagation will be much better than others in AmP. Obtained results are compared with available results of same type of materials.

Keywords: Americium Monopnictides, Coulomb and Born-Mayer Potential, Elastic Constants, Ultrasonic Velocity, Grüneisen Parameters

1. Introduction

Generally, a crystalline material has anisotropic properties. Properties such as thermal expansion and conduction, temperature dependence specific heat, temperature and pressure variation of elastic constants, damping of high frequency acoustic waves and damping of moving dislocations by phonon viscosity are determined by the intrinsic nonlinearity of solids. This emphasizes the importance of non-linear characteristics of solids. Recent developments in the experimental capabilities and theoretical understanding have provided further impetus to the study of the non-linearity in solids [1].

Wave velocity is a key parameter in ultrasonic characterization and can provide information about crystallographic texture. The ultrasonic velocity (V) is related to the elastic constant by the relation $V = \sqrt{C/\rho}$, where C is the relevant elastic constant and ρ is the density of that particular material. Particularly, the elastic constant provides valuable information on stability and stiffness of the materials. The elastic constant of solids also provides a link between the mechanical and dynamical behaviours of crystals and gives important information concerning the nature of forces operating in solids [2].

The Grüneisen parameter is of considerable importance to Earth's scientists, because it sets limitations on the thermoelastic properties of lower mantle [3]. The study of Grüneisen parameters for a solid enable us to describe and discuss various physical properties of a system such as high temperature specific heats of lattice, thermal expansion, thermal conductivity and temperature variation of the elastic constants. The Grüneisen parameters play a significant role in study of thermoelastic properties. It has fundamental importance to the equation of state and related to thermodynamic properties of the solids [4]. The calculation of anharmonic effects in solids such as thermal expansion or the interaction of acoustic and thermal phonons involves Grüneisen parameters, which describe the volume and strain dependence of the lattice vibrational frequencies. In the Debye model, these vibrations are replaced by standing wave modes of a dispersionless elastic continuum. The Grüneisen parameters are then no longer frequency dependent and can be expressed in terms of second- and third- order elastic constants [5].

Yet, the americium monopnictides have not been investigated in detail, but few studies are found elsewhere [6-10]. The ground state and optical properties of ameri-

cium mononpnictides were investigated theoretically by Ghosh *et al.* [6]. The crystal structure of AmAs, AmSb and AmBi were determined by Roddy [7]. The ^{237}Np emission spectra in ^{241}Am : AmO₂, AmAs and AmBi sources have been reported by Friedt *et al.* [8]. The preparation and XRD of AmBi have been made by Gibson and Haire [9]. Petit *et al.* calculated the electronic structure of Am mononpnictides with the help of ab-initio self-interaction-correlated local spin density approximation [10].

Ultrasonic study is non-destructive in nature and is helpful for the determination of inherent properties of materials. The elastic constants of materials are directly related to their microstructure and are used to obtain the Debye average velocity, Grüneisen parameter (GP) and other physical properties; and therefore, these are of great interest in applications where the mechanical strength and durability are important. To the best of our knowledge, no experimental or theoretical reports on ultrasonic velocity and Grüneisen parameters on these materials have been seen in the literature. The grounds mentioned above motivate us to choose these compounds for characterization through ultrasonic non-destructive evaluation technique. For which, we performed theoretical investigation of elastic constants, ultrasonic velocities and Grüneisen parameters in Am mononpnictides along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions at temperature range 100 K - 500 K. The results provide reference data for experimentalists and open a new basis for further study.

2. Theory

The theory is categorized into three phases. In the first phase, temperature dependence of second- and third-order elastic constants (SOEC and TOEC) has been discussed while temperature dependence ultrasonic velocity along different directions has been described in second phase. Temperature dependent Grüneisen parameters along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ orientations have been clarified in the final phase.

2.1. Temperature Dependence of Higher Order Elastic Constants

Elastic properties of a solid are important because they relate to various fundamental solid-state properties such as interatomic potentials, equation of state and phonon spectra. Elastic properties are also linked thermodynamically to the specific heat, thermal expansion, Debye temperature, melting point and Grüneisen parameter. So, it is important to calculate elastic constants of solids. From the calculated elastic constants one can derive the anisotropy in the elastic properties.

The elastic energy density (U) is function of the strain

components.

$$U = F(e_{xx}, e_{yy}, e_{zz}, e_{yz}, e_{zx}, e_{xy}) = F(e_1, e_2, e_3, e_4, e_5, e_6) \quad (1)$$

where e_{ij} (i or j = x, y, z) is component of strain tensor. The second (C_{IJ}) and third (C_{IJK}) order elastic constants of material are defined by following expressions:

$$C_{IJ} = \frac{\partial^2 U}{\partial e_1 \partial e_j}; \quad I \text{ or } J = 1, \dots, 6 \quad (2)$$

$$C_{IJK} = \frac{\partial^3 U}{\partial e_1 \partial e_j \partial e_k}; \quad I \text{ or } J \text{ or } K = 1, \dots, 6 \quad (3)$$

The elastic energy density is well related to interaction potential $\phi(\mathbf{r})$ between atoms. The potential used for evaluation of SOEC and TOEC is taken as sum of Coulomb and Born-Mayer potentials.

$$\phi(\mathbf{r}) = \phi(C) + \phi(B) \quad (4)$$

where $\phi(C)$ is electrostatic/Coulomb potential and $\phi(B)$ is the repulsive/Born-Mayer potential, given as $\phi(C) = \pm(e^2/r)$ and $\phi(B) = A \exp(-r/b)$. Here "e" is electronic charge, "r" is the nearest neighbour distance, "b" is the hardness parameter and "A" is the strength parameter.

According to lattice dynamics developed by Leibfried and Ludwig [11] & Mori and Hiki [12], lattice energy changes with temperature. Hence, the addition of vibrational energy contribution to static elastic constants, one gets second and third order elastic constants (C_{IJ} and C_{IJK}) at required temperature.

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{\text{Vib}} \quad \text{and} \quad C_{IJK} = C_{IJK}^0 + C_{IJK}^{\text{Vib}} \quad (5)$$

where superscript 0 has been used to denote SOEC and TOEC at 0 K (static elastic constants) and superscript Vib has been used to denote vibrational part of SOEC and TOEC at a particular temperature. The expressions of C_{IJ} and C_{IJK} are given in our previous paper [2].

2.2. Orientation Dependence of Ultrasonic Velocities

When sound wave propagates through a crystalline medium, there is three mode of propagation: one longitudinal acoustical (LA) and two transverse acoustical (TA). Thus, there exist three types of velocities as one longitudinal (V_L) and two shear (V_{S1} and V_{S2}). These velocities depend on the direction of propagation of wave [13]. The expressions for direction dependent ultrasonic velocities in cubic crystals are as follows:

Along $\langle 100 \rangle$ crystallographic direction;

$$V_L = \sqrt{\frac{C_{11}}{d}}; \quad V_{S1} = V_{S2} = \sqrt{\frac{C_{44}}{d}} \quad (6)$$

Along $\langle 111 \rangle$ crystallographic direction;

$$V_L = \sqrt{\frac{C_{11} + 2C_{12} + 4C_{44}}{3d}}; V_{S1} = V_{S2} = \sqrt{\frac{C_{11} - C_{12} + C_{44}}{3d}} \quad (7)$$

Along $\langle 110 \rangle$ crystallographic direction;

$$V_L = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2d}}; V_{S1} = \sqrt{\frac{C_{44}}{d}}; V_{S2} = \sqrt{\frac{C_{11} - C_{12}}{d}} \quad (8)$$

The ultrasonic velocities can be worked out using calculated values of second order elastic constants. The Debye average velocity (V_D) is useful for information of Debye temperature and thermal relaxation time of the materials. The following expressions have been used for evaluation of Debye average velocity [13].

$$V_D = \left\{ \begin{array}{l} \left[\frac{1}{3} \left\{ \frac{1}{V_L^3} + \frac{2}{V_{S1}^3} \right\} \right]^{-1/3} \text{ ; along } \langle 100 \rangle \\ \text{and } \langle 111 \rangle \text{ direction} \\ \left[\frac{1}{3} \left\{ \frac{1}{V_L^3} + \frac{1}{V_{S1}^3} + \frac{1}{V_{S2}^3} \right\} \right]^{-1/3} \text{ ; along } \langle 110 \rangle \text{ direction} \end{array} \right\} \quad (9)$$

2.3. Orientation Dependence of Ultrasonic Grüneisen Parameters

A number of anharmonic properties of solids are frequently expressed in terms of Grüneisen parameters that are expressed in quasi-harmonic approximation as diverse weighted averages of Grüneisen tensor of the first order: $\gamma_{\alpha\beta}^j = -\omega_i^{-1} \partial \omega_i(q) / \partial \eta_{\alpha\beta}$. For example, the thermal expansivity is relative to the specific heat weighted $\langle \gamma_{\alpha\beta} \rangle = \sum_{q,i} C_{q,i} \gamma_{\alpha\beta}^j / \sum_{q,i} C_{q,i}$, which is thermal Grüneisen parameter γ . The shear (ultrasonic) Grüneisen parameter can be suitably expressed by thermal conductivity weighted averages of the product $\gamma_{\alpha\beta}^j \gamma_{\gamma\delta}^j$ [14]. Brugger derived expressions for the components of Grüneisen tensor in terms of second- and third- order elastic constants of an anisotropic elastic continuum [15]. These relations permit the above weighted average to be reliably calculated from elastic and thermal data. The comparison of ultrasonic attenuation and non-linear parameters evaluated with help of them, justifies the expression of Grüneisen parameters [16]. Formulae of Grüneisen parameters along different crystallographic directions are given in literature [17].

3. Results and discussion

The second- and third- order elastic constants (SOEC and TOEC) have been evaluated using two basic parameters *i.e.*, lattice parameter and hardness parameter. The lattice pa-

rameters [6-10] for AmN, AmP, AmAs, AmSb and AmBi are 4.825 Å, 5.432 Å, 5.592 Å, 6.003 Å and 6.076 Å respectively and the values of hardness parameter are 0.293 Å, 0.301 Å, 0.302 Å, 0.303 Å and 0.271 Å for AmN, AmP, AmAs, AmSb and AmBi respectively. The computed results of temperature dependent SOEC and TOEC are listed in **Table 1**. We found no experimental/theoretical result of SOEC and TOEC of these materials directly in existing literature. So, we have compared our results with NaCl-type rare-earth monochalcogenides [18].

It is clear from the **Table 1** that, out of nine elastic constants, four (*i.e.*, C_{11} , C_{44} , C_{112} and C_{144}) are decreasing and other four (*i.e.*, C_{12} , C_{111} , C_{166} and C_{123}) are increasing with the temperature while C_{456} is found to be unaffected. The increase or decrease in stiffness constants is due increase or decrease in atomic interaction with temperature. If inter-atomic distance increases or decreases with temperature then interaction potential decreases/increases, which causes decrease or increase in stiffness constants. This type of behaviour has been found already in other NaCl-type materials like gadolinium and cerium mononictides [18,19]. The comparison justifies our calculations of second and third order elastic constants. There are no elastic data as a function of temperature for these compounds in literature. Most simple theories are able to get a reasonable estimate of elastic constants at room temperature only by using experimental parameters. **Table 1** depicts that AmN has highest valued SOEC and TOEC in contrast to other mononictides. Hence mechanical influence of AmN is better than AmP, AmAs, AmSb and AmBi.

The stability of a cubic crystal is expressed in terms of elastic constants as:

$$B_T = \frac{C_{11} + 2C_{12}}{3} > 0, C_{44} > 0 \text{ and } C_S = \frac{C_{11} - C_{12}}{2} > 0.$$

C_{ij} are the conventional elastic constants, B_T is the bulk moduli. The quantities C_{44} and C_S are the shear and tetragonal moduli of a cubic crystal. Estimated values of bulk, shear and tetragonal moduli for AmN, AmP, AmAs, AmSb and AmBi at room temperature are presented in **Tables 1-2** that satisfies the above stability criterion for these materials.

The ultrasonic velocity is a key factor to characterize the properties of material. It is directly related to SOEC and density of that particular material as shown in Eqs. (7-9). The evaluated velocities for longitudinal and shear waves are presented in **Table 3** and the Debye average velocities are shown in **Figures 1-3**.

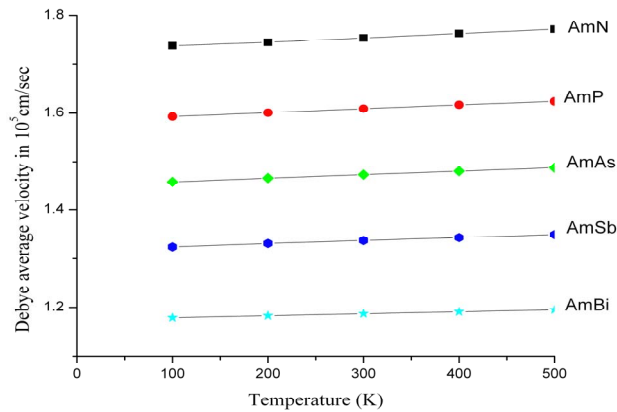
It can be seen that the velocities of the chosen materials along longitudinal and shear waves increase with increase in temperature. The Debye average velocity of these materials is found to increase with temperature. It is also observed that it is large along $\langle 111 \rangle$ direction and

Table 1. Second- and third- order elastic constants of AmY at the temperature range 100 K to 500 K in the unit of 10^{11} Dyne/cm².

Material	Temp (K)	C ₁₁	C ₁₂	C ₄₄	C ₁₁₁	C ₁₁₂	C ₁₂₃	C ₁₄₄	C ₁₆₆	C ₄₅₆
AmN	100	7.15	2.40	2.51	-104.4	-9.87	3.52	4.05	-10.29	4.02
	200	7.30	2.31	2.52	-109.8	-9.56	3.01	4.08	-10.32	4.02
	300	7.50	2.21	2.53	-110.6	-9.23	2.50	4.11	-10.35	4.02
	400	7.71	2.11	2.54	-111.5	-8.90	2.00	4.14	-10.39	4.02
	500	7.93	2.02	2.55	-112.5	-8.60	1.49	4.16	-10.43	4.02
AmP	100	5.28	1.32	1.41	-85.84	-5.35	1.86	2.37	-5.72	2.35
	200	5.42	1.24	1.41	-86.31	-5.05	1.37	2.39	-5.74	2.35
	300	5.59	1.16	1.42	-87.09	-4.74	0.88	2.41	-5.76	2.35
	400	5.77	1.07	1.42	-87.98	-4.42	0.39	2.42	-5.79	2.35
	500	5.96	0.99	1.43	-88.92	-4.10	-0.10	2.44	-5.81	2.35
AmAs	100	4.94	1.16	1.24	-81.50	-4.68	1.61	2.12	-5.04	2.10
	200	5.08	1.08	1.25	-82.02	-4.38	1.12	2.13	-5.05	2.10
	300	5.31	1.00	1.25	-83.60	-4.07	1.07	2.15	-5.08	2.10
	400	5.43	0.92	1.26	-83.83	-3.75	0.14	2.16	-5.10	2.10
	500	5.61	0.84	1.26	-84.77	-3.43	-0.35	2.18	-5.12	2.10
AmSb	100	4.33	0.88	0.96	-73.87	-3.50	1.16	1.66	-3.84	1.65
	200	4.47	0.80	0.96	-74.50	-3.19	0.66	1.68	-3.86	1.65
	300	4.66	0.72	0.96	-75.97	-2.86	0.15	1.69	-3.87	1.65
	400	4.80	0.65	0.97	-76.25	-2.56	0.33	1.70	-3.89	1.65
	500	4.97	0.58	0.97	-77.19	-2.25	0.13	1.71	-3.91	1.65
AmBi	100	5.10	0.76	0.86	-93.99	-2.90	0.83	1.56	-3.38	1.55
	200	5.28	0.67	0.86	-94.83	-2.46	0.12	1.57	-3.39	1.55
	300	5.48	0.58	0.86	-95.96	-2.02	-0.60	1.58	-3.40	1.55
	400	5.69	0.48	0.87	-97.25	-1.57	-1.32	1.59	-3.41	1.55
	500	5.89	0.39	0.87	-98.45	-1.13	-2.03	1.60	-3.43	1.55

Table 2. Bulk moduli (B_T) and tetragonal moduli (C_S) of AmY at room temperature in the unit of 10^{11} Dyne/cm².

Material	B_T	C_S
AmN	3.97	2.64
AmP	2.63	2.22
AmAs	2.44	2.16
AmSb	2.04	1.97
AmBi	2.21	2.45

**Figure 1. Debye average velocity versus temperature along <100> direction.**

is small along <100> direction (**Figures 1-3**). Due to lack of experimental data of these materials for ultrasonic velocities of AmY, we compare our with other B1 structured materials like semiconductors [20], rare-earth monochalcogenides [21,22] and metallic alloys [23]. The order and nature of ultrasonic velocities and Debye average velocity is found to be same. It is clear from **Table 3** that the computed values of ultrasonic velocities are highest in case of AmP. So we can say that the propagation of sound waves through AmP will be better than that of other chosen materials. Hence our approach to compute SOEC and TOEC is logical.

SOEC and TOEC are used to obtain Grüneisen parameters and average squares of the Grüneisen parameters along <100> direction for longitudinal wave over 39 modes and for shear wave 18 modes; along <110> direction for longitudinal wave over 39 modes, for shear wave polarized along <001> direction over 14 modes and for shear wave polarized along <110> direction over 20 modes and along <111> direction for longitudinal wave over 39 modes and for shear wave polarized along <110> direction over 14 modes. The temperature dependent averaged ultrasonic Grüneisen parameters and averaged squares of the Grüneisen parameters are presented in **Table 4**. The value of average Grüneisen parameters is the highest for

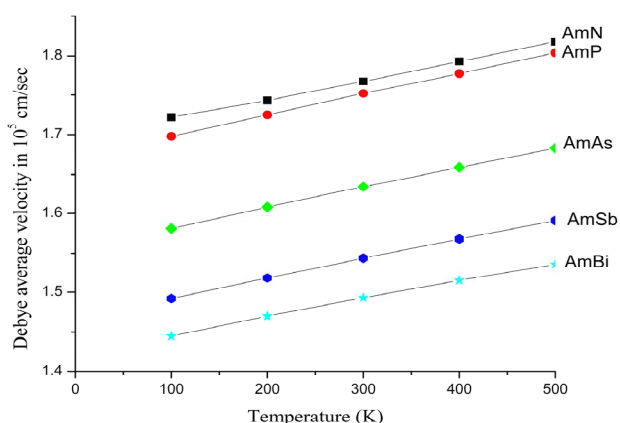


Figure 2. Debye temperature versus temperature along $\langle 111 \rangle$ direction.

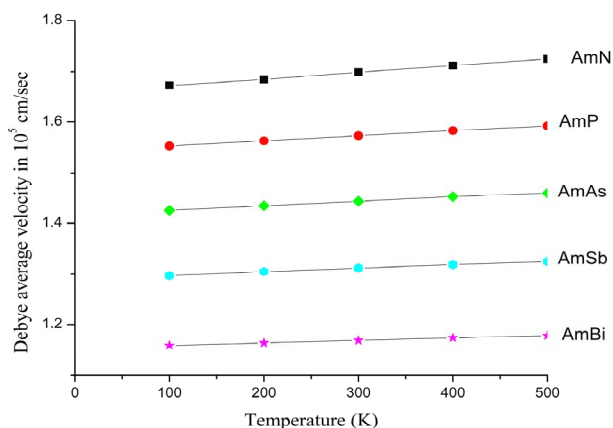


Figure 3. Debye average velocity versus temperature along $\langle 110 \rangle$ direction.

Table 3. Ultrasonic velocities (in 10^5 cm/s) of AmY along different crystallographic directions in the temperature range 100 K - 500 K.

Materials	Directions	Velocity	100 K	200 K	300 K	400 K	500 K	
AmN	$\langle 100 \rangle$	V_L	2.284	2.308	2.339	2.372	2.405	
		$V_{S1} = V_{S2}$	1.353	1.355	1.357	1.360	1.363	
	$\langle 111 \rangle$	V_L	2.312	2.312	2.314	2.317	2.321	
		$V_{S1} = V_{S2}$	1.329	1.351	1.378	1.406	1.434	
	AmP	$\langle 110 \rangle$	V_L	2.305	2.311	2.320	2.331	2.342
			V_{S1}	1.353	1.355	1.357	1.360	1.363
$\langle 100 \rangle$		V_{S2}	1.862	1.909	1.964	2.020	2.076	
		V_L	2.325	2.355	2.392	2.430	2.469	
AmAs	$\langle 111 \rangle$	$V_{S1} = V_{S2}$	1.199	1.201	1.204	1.206	1.208	
		V_L	2.145	2.146	2.101	2.153	2.157	
	$\langle 110 \rangle$	$V_{S1} = V_{S2}$	1.346	1.378	1.410	1.432	1.475	
		V_L	2.188	2.199	2.211	2.225	2.238	
	AmSb	$\langle 110 \rangle$	V_{S1}	1.199	1.201	1.204	1.206	1.208
			V_{S2}	2.015	2.069	2.131	2.193	2.254
$\langle 100 \rangle$		V_L	2.177	2.209	2.259	2.284	2.321	
		$V_{S1} = V_{S2}$	1.092	1.094	1.097	1.098	1.100	
AmBi	$\langle 111 \rangle$	V_L	1.973	1.976	1.979	1.983	1.986	
		$V_{S1} = V_{S2}$	1.261	1.293	1.325	1.357	1.388	
	$\langle 110 \rangle$	V_L	2.023	2.035	2.048	2.061	2.074	
		V_{S1}	1.092	1.094	1.097	1.098	1.100	
AmSb	$\langle 110 \rangle$	V_{S2}	1.905	1.961	2.036	2.081	2.140	
		V_L	2.083	2.117	2.162	2.194	2.233	
	$\langle 100 \rangle$	$V_{S1} = V_{S2}$	0.979	0.981	0.982	0.984	0.986	
		V_L	1.815	1.818	1.821	1.824	1.828	
	$\langle 111 \rangle$	$V_{S1} = V_{S2}$	1.207	1.240	1.273	1.306	1.337	
		V_L	1.883	1.896	1.909	1.923	1.936	
AmBi	$\langle 110 \rangle$	V_{S1}	0.979	0.981	0.982	0.984	0.986	
		V_{S2}	1.860	1.918	1.987	2.039	2.099	
	$\langle 100 \rangle$	V_L	2.079	2.115	2.154	2.195	2.195	
		$V_{S1} = V_{S2}$	0.854	0.855	0.857	0.858	0.859	
	$\langle 111 \rangle$	V_L	1.682	1.684	1.687	1.689	1.689	
		$V_{S1} = V_{S2}$	1.204	1.239	1.274	1.307	1.307	
$\langle 110 \rangle$	V_L	1.786	1.799	1.814	1.828	1.828		
	V_{S1}	0.854	0.855	0.857	0.858	0.859		
		V_{S2}	1.917	1.976	2.038	2.100	2.100	

Table 4. Ultrasonic Grüneisen parameters of AmY along different crystallographic directions in the temperature range 100 K - 500 K.

Material	Grüneisen parameters	100 K	200 K	300 K	400 K	500 K
Ultrasonic longitudinal wave propagates along <100>						
AmN	$\langle \gamma_i^j \rangle$	0.459	0.444	0.429	0.414	0.400
	$\langle (\gamma_i^j)^2 \rangle$	1.768	1.674	1.576	1.487	1.407
AmP	$\langle \gamma_i^j \rangle$	0.453	0.437	0.419	0.403	0.389
	$\langle (\gamma_i^j)^2 \rangle$	1.976	1.863	1.751	1.651	1.561
AmAs	$\langle \gamma_i^j \rangle$	0.455	0.436	0.416	0.402	0.387
	$\langle (\gamma_i^j)^2 \rangle$	2.048	1.923	1.791	1.701	1.608
AmSb	$\langle \gamma_i^j \rangle$	0.455	0.436	0.417	0.399	0.383
	$\langle (\gamma_i^j)^2 \rangle$	2.207	2.067	1.947	1.824	1.725
AmBi	$\langle \gamma_i^j \rangle$	0.463	0.441	0.421	0.402	0.385
	$\langle (\gamma_i^j)^2 \rangle$	2.670	2.507	2.360	2.230	2.119
Ultrasonic shear wave propagates along <100> and polarized along <100> direction						
AmN	$\langle (\gamma_i^j)^2 \rangle$	0.120	0.118	0.116	0.115	0.113
AmP	$\langle (\gamma_i^j)^2 \rangle$	0.119	0.118	0.117	0.116	0.115
AmAs	$\langle (\gamma_i^j)^2 \rangle$	0.120	0.119	0.117	0.117	0.116
AmSb	$\langle (\gamma_i^j)^2 \rangle$	0.122	0.121	0.120	0.119	0.119
AmBi	$\langle (\gamma_i^j)^2 \rangle$	0.129	0.128	0.128	0.127	0.127
Ultrasonic longitudinal wave propagates along <111>						
AmN	$\langle \gamma_i^j \rangle$	-0.689	-0.660	-0.630	-0.603	-0.577
	$\langle (\gamma_i^j)^2 \rangle$	2.167	1.994	1.825	1.676	1.546
AmP	$\langle \gamma_i^j \rangle$	-0.710	-0.677	-0.644	-0.615	-0.588
	$\langle (\gamma_i^j)^2 \rangle$	2.275	2.072	1.883	1.720	1.577
AmAs	$\langle \gamma_i^j \rangle$	-0.719	-0.683	-0.646	-0.619	-0.591
	$\langle (\gamma_i^j)^2 \rangle$	2.333	2.112	1.896	1.743	1.596
AmSb	$\langle \gamma_i^j \rangle$	-0.737	-0.698	-0.663	-0.630	-0.601
	$\langle (\gamma_i^j)^2 \rangle$	2.456	2.209	1.999	1.807	1.648
AmBi	$\langle \gamma_i^j \rangle$	-0.789	-0.747	-0.708	-0.672	-0.641
	$\langle (\gamma_i^j)^2 \rangle$	2.859	2.565	2.309	2.091	1.906
Ultrasonic shear wave propagates along <111> and polarized along <110> direction						
AmN	$\langle (\gamma_i^j)^2 \rangle$	1.9468	1.881	1.810	1.744	1.683
AmP	$\langle (\gamma_i^j)^2 \rangle$	2.286	2.202	2.117	2.039	1.969
AmAs	$\langle (\gamma_i^j)^2 \rangle$	2.3838	2.290	2.187	2.120	2.048
AmSb	$\langle (\gamma_i^j)^2 \rangle$	2.6036	2.499	2.416	2.317	2.242
AmBi	$\langle (\gamma_i^j)^2 \rangle$	3.2101	3.098	2.998	2.912	2.842
Ultrasonic longitudinal wave propagates along <110>						
AmN	$\langle \gamma_i^j \rangle$	-0.774	-0.748	-0.720	-0.694	-0.669
	$\langle (\gamma_i^j)^2 \rangle$	2.302	2.154	2.007	1.875	1.758
AmP	$\langle \gamma_i^j \rangle$	-0.760	-0.730	-0.699	-0.671	-0.644
	$\langle (\gamma_i^j)^2 \rangle$	2.488	2.324	2.168	2.031	1.911
AmAs	$\langle \gamma_i^j \rangle$	-0.761	-0.729	-0.691	-0.667	-0.639
	$\langle (\gamma_i^j)^2 \rangle$	2.569	2.392	2.214	2.089	1.967
AmSb	$\langle \gamma_i^j \rangle$	-0.760	-0.724	-0.689	-0.657	-0.628
	$\langle (\gamma_i^j)^2 \rangle$	2.758	2.565	2.404	2.243	2.114
AmBi	$\langle \gamma_i^j \rangle$	0.765	-0.726	-0.687	-0.652	-0.619
	$\langle (\gamma_i^j)^2 \rangle$	3.361	3.143	2.951	2.786	2.645
Ultrasonic shear wave propagates along <110> and polarized along <001> direction						
AmN	$\langle (\gamma_i^j)^2 \rangle$	0.126	0.122	0.119	0.115	0.112
AmP	$\langle (\gamma_i^j)^2 \rangle$	0.104	0.101	0.099	0.097	0.095
AmAs	$\langle (\gamma_i^j)^2 \rangle$	0.101	0.098	0.095	0.094	0.092
AmSb	$\langle (\gamma_i^j)^2 \rangle$	0.095	0.093	0.091	0.089	0.088
AmBi	$\langle (\gamma_i^j)^2 \rangle$	0.088	0.087	0.086	0.084	0.083
Ultrasonic shear wave propagates along <110> and polarized along <110> direction						
AmN	$\langle (\gamma_i^j)^2 \rangle$	2.852	2.749	2.638	2.531	2.432
AmP	$\langle (\gamma_i^j)^2 \rangle$	3.037	3.236	3.097	2.968	2.851
AmAs	$\langle (\gamma_i^j)^2 \rangle$	3.524	3.372	3.201	3.089	2.968
AmSb	$\langle (\gamma_i^j)^2 \rangle$	3.865	3.693	3.553	3.388	3.261
AmBi	$\langle (\gamma_i^j)^2 \rangle$	4.820	4.634	4.467	4.324	4.206

AmN along $\langle 100 \rangle$ direction and the lowest for AmBi along $\langle 111 \rangle$ direction for longitudinal waves, while averaged square Grüneisen parameters is the highest for AmBi along $\langle 110 \rangle$ direction in which shear wave polarized along $\langle 110 \rangle$ direction, and the lowest for AmBi in which shear wave polarized along $\langle 001 \rangle$ direction as shown in **Table 4**. Hence we can say that AmN is the best for longitudinal wave propagation along $\langle 100 \rangle$ direction and AmBi would be the best for shear wave propagation. It is found that obtained values of Grüneisen parameters and average squares of the Grüneisen parameters are decreasing with the temperature. This is due to adjustment of SOEC and TOEC for different modes. This type of nature is also found in other B1 structured materials like rare-earth monochalcogenides [21,22,24], semiconductors [20] and metallic alloys [23]. It establishes that properties of these materials are very similar to either a semiconductor or metals.

4. Conclusions

On the basis of analysis of above result, we can say that:

1) We have used the Coulomb and Born-Mayer potential having two basic parameters *i.e.*, lattice parameter and hardness parameter to compute SOEC and TOEC. Evaluated values of SOEC and TOEC have been compared with available B1 structured materials, which are near to agreement, hence our approach to calculation appears to justify.

2) SOEC and TOEC of AmN are the highest so mechanical properties will be better than other AmY.

3) SOEC and TOEC have been used to find out the ultrasonic velocities for longitudinal and shear waves, Debye average velocity and Grüneisen parameters in AmY.

4) Ultrasonic velocity is found to be highest for AmN along all chosen direction, so AmN will be most suitable candidate for wave propagation.

5) AmN is the best for longitudinal wave propagation along $\langle 100 \rangle$ direction and AmBi is the best for thermal purposes, because Grüneisen parameters are most sensitive to temperature.

Due to absence of experimental information on ultrasonic properties of these mononictides, no straight evaluation have been made, yet, on the basis of agreement values of elastic constants, ultrasonic velocities and Grüneisen parameters, we conclude that current approach is justified and obtained results will be useful for finding various theoretical, experimental investigations like ultrasonic attenuation, non-linearity parameters, ultrasonic measurements, polarizing microscopy, solid state NMR, SEM, TEM; and for scientific world and society.

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