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 <100>, <110> and <111> 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 \( V = \sqrt{\frac{C}{\rho}} \), where C is the relevant elastic constant and \( \rho \) 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 monopnictides were investigated theoretically by Ghosh et al. [6]. The crystal structure of AmAs, AmSb and AmBi were determined by Roddy [7]. The $^{237}\text{Np}$ emission spectra in $^{241}\text{Am}: \text{AmO}_2$, 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 monopnictides 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 monopnictides along $<100>$, $<110>$ and $<111>$ 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 $<100>$, $<110>$ and $<111>$ 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.

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

where $e_i$ (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:

$$C_{ij} = \frac{\delta^2 U}{\delta e_i \delta e_j}; \text{ if } i = j, 1, \ldots, 6$$  \hspace{1cm} (2)

$$C_{ijk} = \frac{\delta^2 U}{\delta e_i \delta e_j \delta e_k}; \text{ if } i \neq j \neq k, 1, \ldots, 6$$  \hspace{1cm} (3)

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

$$\phi(r) = \phi(C) + \phi(B)$$  \hspace{1cm} (4)

where $\phi(C)$ is electrostatic/Coulomb potential and $\phi(B)$ is the repulsive/Born-Mayer potential, given as $\phi(C) = \pm \left(\frac{e^2}{r}\right)$ 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.

$$C_{ij} = C_{ij}^0 + C_{ij}^{Vib} \quad \text{and} \quad C_{ijk} = C_{ijk}^0 + C_{ijk}^{Vib}$$  \hspace{1cm} (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 $<100>$ crystallographic direction;

$$V_L = \sqrt{\frac{C_{11}}{d}}; \quad V_{S1} = V_{S2} = \sqrt{\frac{C_{44}}{d}}$$  \hspace{1cm} (6)

Along $<111>$ crystallographic direction;
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].

\[
V_L = \sqrt{\frac{C_{11} + 2C_{12} + 4C_{44}}{3d}}; \quad V_S = \sqrt{\frac{C_{11} - C_{12} + 4C_{44}}{3d}}
\]  
\[
V_L = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2d}}; \quad V_S = \sqrt{\frac{C_{44}}{d}}; \quad V_S = \sqrt{\frac{C_{11} - C_{12}}{d}}
\]

Along <110> crystallographic direction;

\[
V_L = \left[ \frac{1}{3} \left( \frac{1}{V_L} + \frac{2}{V_S} \right) \right]^{1/3}; \quad \text{along <100> direction}
\]

\[
= \left[ \frac{1}{3} \left( \frac{1}{V_L} + \frac{1}{V_S} \right) \right]^{1/3}; \quad \text{along <110> direction}
\]

2.3. Orientation Dependence of Ultrasonic Grüneneisen Parameters

A number of anharmonic properties of solids are frequently expressed in terms of Grüneneisen parameters that are expressed in quasiharmonic approximation as diverse weighted averages of Grüneneisen tensor of the first order: 

\[
\gamma_{d\beta} = -\alpha_i \frac{\partial \omega_i(q)}{\partial n_{d\beta}}. 
\]

For example, the thermal expansivity is relative to the specific heat weighted

\[
\gamma_{d\beta} = \sum_{q,i} C_{q,i} \gamma_{q,i} + \sum_{q,i} C_{q,i}. 
\]

Brugger derived expressions for the components of Grüneneisen 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 suitably expressed by thermal conductivity weighted averages of the product \( \gamma_{d\beta} \gamma_{q,i} \) [14].

\[
B_i = C_{11} + 2C_{12} > 0, \quad C_{44} > 0 \quad \text{and} \quad C_S = C_{11} - C_{12} > 0.
\]

C_{11} are the conventional elastic constants, \( B_i \) 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 <111> 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.

<table>
<thead>
<tr>
<th>Material</th>
<th>Temp (K)</th>
<th>C₁₁</th>
<th>C₁₂</th>
<th>C₄₄</th>
<th>C₁₁₁</th>
<th>C₁₁₂</th>
<th>C₁₂₃</th>
<th>C₁₄₄</th>
<th>C₁₆₆</th>
<th>C₄₅₆</th>
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<td></td>
<td>100</td>
<td>7.15</td>
<td>2.40</td>
<td>2.51</td>
<td>-104.4</td>
<td>-9.87</td>
<td>3.52</td>
<td>4.05</td>
<td>-10.29</td>
<td>4.02</td>
</tr>
<tr>
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<td>2.31</td>
<td>2.52</td>
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<td>-9.56</td>
<td>3.01</td>
<td>4.08</td>
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<td>4.02</td>
</tr>
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<td>2.53</td>
<td>-110.6</td>
<td>-9.23</td>
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<td>4.11</td>
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<tr>
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<td>400</td>
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<td>4.14</td>
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<td>1.86</td>
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<td>1.42</td>
<td>-87.09</td>
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<td>-5.05</td>
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<td>1.00</td>
<td>1.25</td>
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<td>-5.08</td>
<td>2.10</td>
</tr>
<tr>
<td></td>
<td>400</td>
<td>5.43</td>
<td>0.92</td>
<td>1.26</td>
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<td>-3.75</td>
<td>0.14</td>
<td>2.16</td>
<td>-5.10</td>
<td>2.10</td>
</tr>
<tr>
<td>AmSb</td>
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<td>0.96</td>
<td>-73.87</td>
<td>-3.50</td>
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<td>2.16</td>
<td>-3.84</td>
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</tr>
<tr>
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<td>0.96</td>
<td>-74.50</td>
<td>-3.19</td>
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<td>1.68</td>
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<td></td>
<td>300</td>
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<td>0.96</td>
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<td>1.70</td>
<td>-3.89</td>
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<td></td>
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<td>0.97</td>
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<td>0.13</td>
<td>1.71</td>
<td>-3.91</td>
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<tr>
<td>AmBi</td>
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<td>0.76</td>
<td>0.86</td>
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<td>1.57</td>
<td>-3.39</td>
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<td>0.50</td>
<td>1.60</td>
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</table>

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

<table>
<thead>
<tr>
<th>Material</th>
<th>$B_T$</th>
<th>$C_S$</th>
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<tbody>
<tr>
<td>AmN</td>
<td>3.97</td>
<td>2.64</td>
</tr>
<tr>
<td>AmP</td>
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<td>2.22</td>
</tr>
<tr>
<td>AmAs</td>
<td>2.44</td>
<td>2.16</td>
</tr>
<tr>
<td>AmSb</td>
<td>2.04</td>
<td>1.97</td>
</tr>
<tr>
<td>AmBi</td>
<td>2.21</td>
<td>2.45</td>
</tr>
</tbody>
</table>

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 <111> direction.

Figure 3. Debye average velocity versus temperature along <110> direction.

Table 3. Ultrasonic velocities (in $10^6$ cm/s) of AmY along different crystallographic directions in the temperature range 100 K - 500 K.

<table>
<thead>
<tr>
<th>Materials</th>
<th>Directions</th>
<th>Velocity</th>
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<th>200 K</th>
<th>300 K</th>
<th>400 K</th>
<th>500 K</th>
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<td>$V_L$</td>
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<td>1.357</td>
<td>1.360</td>
<td>1.363</td>
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<tr>
<td></td>
<td>&lt;110&gt;</td>
<td>$V_L$</td>
<td>2.312</td>
<td>2.312</td>
<td>2.314</td>
<td>2.317</td>
<td>2.321</td>
</tr>
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<td></td>
<td>&lt;110&gt;</td>
<td>$V_S_1$</td>
<td>1.329</td>
<td>1.351</td>
<td>1.378</td>
<td>1.406</td>
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<td>$V_S_2$</td>
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<td>$V_S_3$</td>
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<td>1.360</td>
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<td>1.204</td>
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<td>$V_L$</td>
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<td>2.101</td>
<td>2.153</td>
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Table 4. Ultrasonic Grüneisen parameters of AmY along different crystallographic directions in the temperature range 100 K - 500 K.

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AmN along <100> direction and the lowest for AmBi along <111> direction for longitudinal waves, while averaged square Grüneisen parameters is the highest for AmBi along <110> direction in which shear wave polarized along <110> direction, and the lowest for AmBi in which shear wave polarized along <001> direction as shown in Table 4. Hence we can say that AmN is the best for longitudinal wave propagation along <100> 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 <100> 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 monopnictides, 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.

5. Acknowledgements

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6. References


