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Acoustic Wave Propagation in Hexagonal MgTe, ZnTe and CdTe Compounds

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ABSTRACT

The acoustic wave propagation in the hexagonal structured materials MgTe, ZnTe and CdTe have been studied at room temperature. In this paper, the orientation dependence of three types of acoustic wave velocity and Debye average velocity have been calculated using second order elastic constants. The six second order elastic constants are calculated for theses materials at 300 K using Lenard-Jones Potential. An anomalous behaviour in orientation dependent acoustic wave velocity is obtained which is due to the combined effect of elastic constants and density. These velocity data are important for their structural information and to differentiate them from third group nitrides and laves-phase compounds. Obtained results, together with other well known physical properties, may expand future prospects for the applications and study of these materials.

Keywords: Elastic constants; longitudinal waves, surface waves

1. INTRODUCTION

It is well known that II-VI semiconductor compounds have a large optical gap, but the feasibility of green-blue opto-electronic devices based on these materials has been demonstrated by Hasse et al. [1]. Due to their wide direct band gap, the electronic properties of compounds such ZnTe and CdTe, appear to be rather promising for applications in optical devices. Technological and theoretical interest in II-VI compound and their alloys is due to its appealing properties in electro-optical and electron acoustic devices [2-4]. Experimentally, MgTe, ZnTe and CdTe are found to have room temperature direct bad gaps of 3.4, 2.4 and 1.5 eV, respectively [5]. This makes them excellent candidates for low cast thin film of high efficiency multi junction solar cell materials to complement existing CdTe and Cu(In,Ga)Se_2 technologies [6]. Their potential for high efficiency solid-state light-emission devices has also been noted [7, 8].

There are three types of acoustic mode lattice vibration: one longitudinal acoustic and two transverse acoustical for hexagonal and cubic structured materials [9-10]. Hence, there are three types of acoustic wave velocities for each direction of propagation of wave, which are well related to second order elastic constants. The one longitudinal sound velocity and one transverse sound velocity for ZnTe and CdTe has been reported in [11] but all the three type of acoustic wave velocity of these all materials are not reported in literature. Therefore in this paper, we have calculated the three types of acoustic wave velocities of hexagonal structured MgTe,, ZnTe and CdTe compounds at room temperature for each direction of propagation of wave using the second order elastic constants that are important for surface and structural study of these materials. The six second order elastic constants are calculated using Lenard-Jones Potential that is many body interaction potential. The calculated ultrasonic parameters are discussed with related thermophysical properties for the characterization of the chosen semiconductors. The obtained results are interesting for the characterization of these materials.

2. THEORY

In the present investigation, the theory is divided into two parts:

2.1 Second-and third order Elastic constants

The second (C_{IJ}) and third (C_{IJK}) order elastic constants of material are defined by following expressions.

$$C_{IJ} = \frac{\partial^2 U}{\partial e_I \partial e_J}; \qquad I \text{ or } J = 1,......6 \tag{1}$$

$$C_{IJK} = \frac{\partial^3 U}{\partial e_I \partial e_J \partial e_K}; \; I \text{ or } J \text{ or } K = 1,\ldots\ldots 6 \tag{2}$$

where, U is elastic energy density , $e_I = e_{ij}$ (i or j = x, y, z, I=1, ...6) is component of strain tensor. Eqs (1) and (2) leads six second and ten third order elastic constants (SOEC and TOEC) for the hexagonal close packed structure materials [12, 13].

$$\left.\begin{array}{ll} C_{11} = 24.1\, p^4 C' & C_{12} = 5.918\, p^4 C' \\ C_{13} = 1.925\, p^6 C' & C_{33} = 3.464\, p^8 C' \\ C_{44} = 2.309\, p^4 C' & C_{66} = 9.851\, p^4 C' \end{array}\right\} \tag{3a}$$

$$\left.\begin{array}{ll} C_{111} = 126.9\, p^2 B + 8.853\, p^4 C' & C_{112} = 19.168\, p^2 B - 1.61\, p^4 C' \\ C_{113} = 1.924\, p^4 B + 1.155\, p^6 C' & C_{123} = 1.617\, p^4 B - 1.155\, p^6 C' \\ C_{133} = 3.695\, p^6 B & C_{155} = 1.539\, p^4 B \\ C_{144} = 2.309\, p^4 B & C_{344} = 3.464\, p^6 B \\ C_{222} = 101.039\, p^2 B + 9.007\, p^4 C' & C_{333} = 5.196\, p^8 B \end{array}\right\} \tag{3b}$$

where p = c/a: axial ratio; $C' = \chi a / p^5$; $B = \psi a^3 / p^3$; $\chi = (1/8)[\{nb_0 (n - m)\}/\{a^{n+4}\}]$

$\psi = -\chi/\{6 a^2 (m + n + 6)\}$; m, n=integer quantity; b_0=Lennard Jones parameter.

2.2 Acoustic wave velocity in hexagonal structured crystal

The anisotropic behaviour of the material can be understood with the knowledge of ultrasonic velocity because the velocity is related to the second order elastic constants [13]. On the basis of mode of atomic vibration, there are three types of velocities (longitudinal, quasi shear and shear) in acoustical region [14]. These velocities vary with the direction of propagation of wave from the unique axis of hexagonal structured crystal [15]. The ultrasonic velocities as a function of angle between direction of propagation and unique axis for hexagonal structured materials are [16]:

$$V_L^2 = \{C_{33} \mathrm{Cos}^2\theta + C_{11} \mathrm{Sin}^2\theta + C_{44} + \{[C_{11} \mathrm{Sin}^2\theta - C_{33} \mathrm{Cos}^2\theta + C_{44} (\mathrm{Cos}^2\theta - \mathrm{Sin}^2\theta)]^2$$

$$+ 4\,\mathrm{Cos}^2\theta\, \mathrm{Sin}^2\theta\, (C_{13} + C_{44})^2\}^{1/2}\}/2\rho \tag{4}$$

$$V_{S1}^{2} = \{C_{33}\,\mathrm{Cos}^{2}\theta + C_{11}\,\mathrm{Sin}^{2}\theta + C_{44} - \{[C_{11}\,\mathrm{Sin}^{2}\theta - C_{33}\,\mathrm{Cos}^{2}\theta + C_{44}\,(\mathrm{Cos}^{2}\theta - \mathrm{Sin}^{2}\theta)]^{2} + 4\,\mathrm{Cos}^{2}\theta\,\mathrm{Sin}^{2}\theta\,(C_{13} + C_{44})^{2}\}^{1/2}\}/2\rho \tag{5}$$

$$V_{S2}^{2} = \{C_{44}\,\mathrm{Cos}^{2}\theta + C_{66}\,\mathrm{Sin}^{2}\theta\}/\rho \tag{6}$$

where V_L, V_{S1} and V_{S2} are longitudinal, quasi shear and pure shear wave ultrasonic velocities. Variables 'ρ' and 'θ' represent the density of the material and angle with the unique axis of the crystal respectively. The Debye temperature (T_D) is an important physical parameter for the characterization of materials, which is well related to the Debye average velocity (V_D).

$$T_D = \frac{\hbar\, V_D\,(6\pi^{2} n_a)^{1/3}}{K_B} \tag{7}$$

here $$V_D = \left\{\frac{1}{3}\left(\frac{1}{V_L^{3}} + \frac{1}{V_{S1}^{3}} + \frac{1}{V_{S2}^{3}}\right)\right\}^{-1/3} \tag{8}$$

where $\hbar$ is quantum of action and is equal to Planck's constant divided by 2π; K_B is Boltzmann Constant; n_a is atom concentration.

3. RESULTS AND DISCUSSION

3.1 Higher order elastic constants

The unit cell parameters 'a' (basal plane parameter) and 'p' (axial ratio) for MgTe, ZnTe and CdTe are 4.51Å, 4.28Å, 4.58Å and 1.627, 1.637, 1.635 [17, 18] respectively. The value of m and n for chosen materials are 6 and 7. The values of b_0 for these materials are 2.2×10^{-63} erg cm^{7}, 1.4×10^{-63} erg cm^{7} and 2.0×10^{-63} erg cm^{7} respectively. The SOEC and TOEC have been calculated for these materials using Eq. (3) and are presented in Table 1.

Table 1. Second and third order elastic constants (SOEC and TOEC) & bulk modulus (B) in the unit of $10^{10}Nm^{-2}$ of materials at room temperature.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B
MgTe	8.118	1.993	1.716	8.176	2.059	3.184	3.917
ZnTe	8.731	2.144	1.869	9.013	2.242	3.424	4.249
CdTe	6.396	1.571	1.366	6.570	1.638	2.508	3.107
MgTe[17]							3.91
ZnTe[19]	8.56	3.70	3.00	9.26	2.02	2.43	
CdTe[19]	6.22	3.59	2.91	6.89	1.16	1.31	

	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{344}	C_{144}	C_{155}	C_{222}	C_{333}
MgTe	-132.38	-20.99	-4.40	-5.60	-27.62	-25.89	-6.52	-4.35	-104.74	-102.81
ZnTe	-142.37	-22.57	-4.79	-6.09	-30.44	-28.54	-7.10	-4.73	-112.65	-114.71
CdTe	-104.30	-16.54	-3.50	-4.45	-22.19	-20.80	-5.19	-3.46	-82.53	-83.42

The elastic constants of the material are important, since they are related to hardness and therefore of interest in applications where mechanical strength and durability are important. Also, the second order elastic constants are used for the determination of the ultrasonic attenuation and related parameters. It is obvious from Table 1 that, there is good agreement between the present and reported theoretical and experimental second order elastic constants of ZnTe and CdTe [19]. The bulk modulus (B) for these compounds can be calculated with the formula $B= 2(C_{11}+ C_{12}+ 2C_{13} + C_{33}/2)/9$. The evaluated B for these compounds is presented in Table 1. It is obvious from Table 1 that, there is good agreement between the present and reported theoretical bulk modulus of MgTe [17]. The Debye temperature Also, the comparison can be made with the value of Debye temperature ZnTe. The present value of Debye temperature for ZnTe is 218.4 ^{0}K, calculated using second order elastic constants. The Debye temperature experimentally determined by Lee [20] is 225.3 ^{0}K. Thus our theoretical approach for the calculation of second order elastic constants for hexagonal structured materials at room temperature is well justified. However, third order elastic constants are not compared due to lack of data in the literature but the negative third order elastic constants are found our previous papers for hexagonal structure materials [12, 13, 15, 16]. Hence applied theory for the evaluation of higher order elastic constants at room temperature is justified.

3.2. Acoustical wave velocity and allied parameters

The computed orientation dependent ultrasonic wave velocities and Debye average velocities at 300 K are shown in Figs.1–4. Figs.1–3 show that the velocities V_L and V_{S1} have minima and maxima respectively at 45° with the unique axis of the crystal while V_{S2} increases with the angle from the unique axis. The combined effect of SOEC and density is reason for abnormal behaviour of angle dependent velocities.

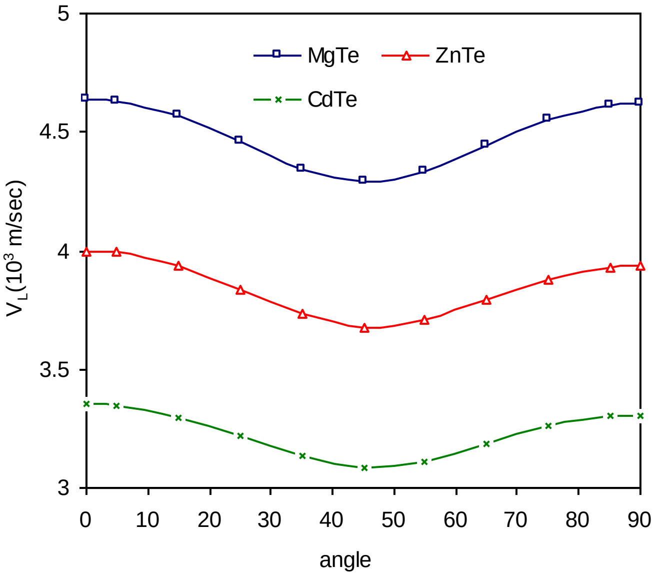

Figure1. V_L vs angle with unique axis of crystal

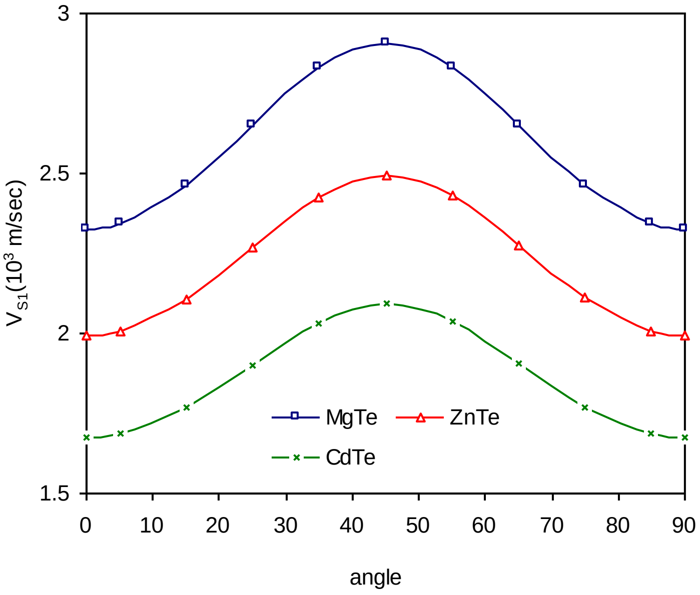

Figure2. V_{S1} vs angle with unique axis of crystal

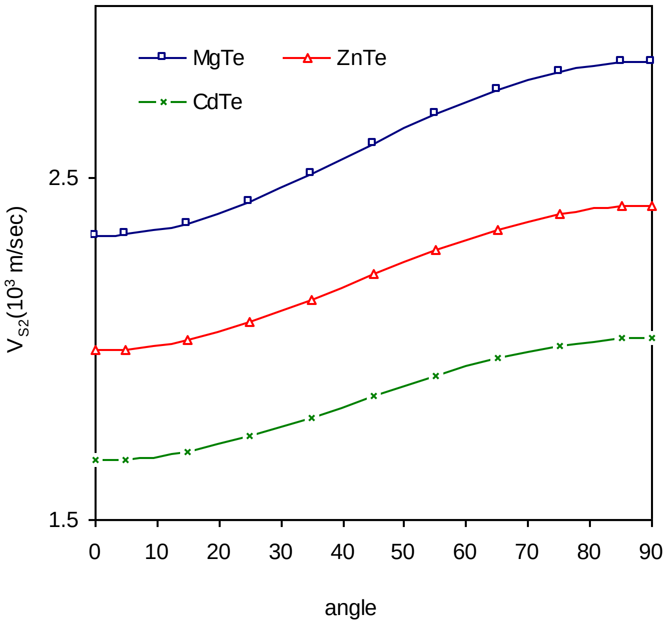

Figure3. V_{S2} vs angle with unique axis of crystal

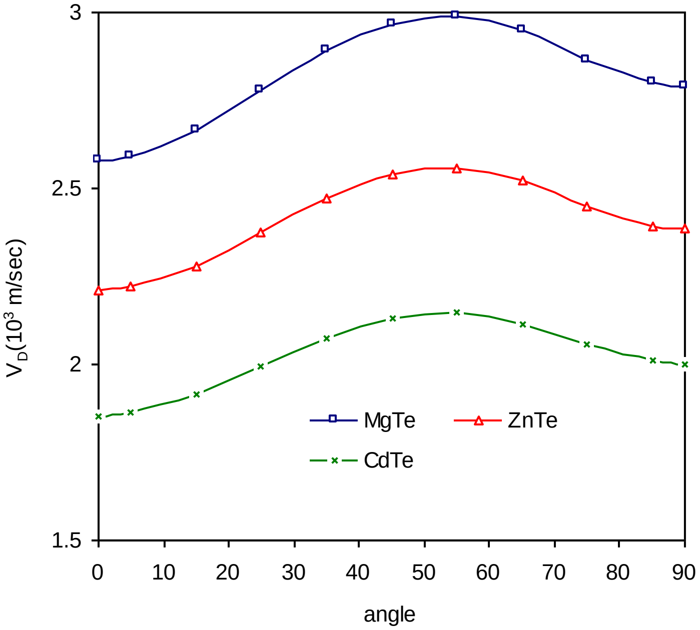

Figure4. V_D vs angle with unique axis of crystal

The nature of the angle dependent velocity curves in the present work is found similar as that for heavy rare-earth metals, third group nitrides, laves-phase compounds and other hexagonal wurtzite structured materials [12, 13, 15, 16, 22]. The chosen materials have shown similar properties with their crystal structure. The comparative study of ultrasonic velocities is presented in Table 2.

Table 2: Comparative velocities (in 10^3 m/s) of ZnTe, CdTe compounds.

	Velocity	Present work theoretical	Bijalwan et al.[11] theoretical
ZnTe	long.	3.99	3.58
	shear	2.00	2.74
CdTe	long.	3.35	3.47
	shear	1.67	2.93

Hence values of velocities are in good agreement with experimental/theoretical values. Thus the angle dependencies of the velocities in these materials are justified.

Figs.1–3 indicate that the magnitude of acoustical velocity is larger for MgTe and smaller for CdTe. . The respective smaller magnitude of acoustical velocity in CdTe is due to its higher gravitational density.

Debye average velocity (V_D) of these materials is increasing with the angle and has maxima at 55° at 300 K (Fig. 4). Since V_D is calculated using V_L, V_{S1} and V_{S2} [12, 16], therefore the angle variation of V_D is influenced by the constituent ultrasonic velocities. The maximum V_D at 55° is due to a significant increase in longitudinal and pure shear (V_{S2}) wave velocities and a decrease in quasi-shear (V_{S1}) wave velocity. Thus it can be concluded that when a sound wave travels at 55° with the unique axis of these crystals then the average sound wave velocity is maximum.

The evaluated Debye temperature for MgTe, ZnTe and CdTe is 241.9 ^{0}K, 218.4 ^{0}K and 182 ^{0}K respectively. The Debye temperature experimentally determined by Lee [20] is 225.3 ^{0}K. Debye (average) sound velocity is useful for the evaluation of Debye temperature [14] and the Debye temperature is well related to specific heat per unit volume and thermal energy density [22]. The Debye average velocity for MgTe, ZnTe and CdTe is $2.578\text{x}10^3$ m/s, $2.210\text{x}10^3$ m/s and $1.885\text{x}10^3$ m/s respectively, which has a similar tend as the Debye temperature. Thus the preset average sound velocity directly correlates with the Debye temperature, specific heat and thermal energy density of these materials. The Debye average velocity has a minimum value for CdTe in comparison to other two materials along every direction of propagation (Fig. 4). This indicates that MgTe is much stable than CdTe due to the large average sound velocity [16].

The ratio $A= 4\ C_{44} / (C_{11}+ C_{33}- 2C_{13})$ is the measure of elastic anisotropy in the crystal. The value of 'A' for MgTe, ZnTe and CdTe is 0.643, 0.642 and 0.641 respectively. A comparison of these anisotropy values with those of GaN, AlN, InN (III group nitride-semiconductor) [23, 24] implies that the elastic anisotropy of these materials is lower than the III group nitrides. Hence, by proposing a low value of anisotropy, these materials favour instability in comprasion to those of III group nitrides.

4. CONCLUSIONS

On the basis of above discussion, we conclude following points:

- Our theory of higher order elastic constants is justified for the hexagonal structured materials.

- Although, the nature of angle dependency of acoustical velocity in these materials is quite similar to that of laves phase compounds and third group nitrides but they favour instability due to lower anisotropy.
- All elastic constants and density are mainly the affecting factor for anomalous behaviour of acoustical velocity in these materials.
- The average sound velocity is a direct consequence of Debye temperature, specific heat and thermal energy density of these compounds.
- The mechanical properties of MgTe are better than those of CdTe, because CdTe has low ultrasonic velocities and thus high attenuation.

Thus obtained results in the present work can be used for further investigations, general and industrial applications. Our theoretical approach is valid for ultrasonic characterization of these compounds at room temperature. The acoustic behavior in these materials as discussed above shows important microstructural characteristic feature, which are well connected to thermoelectric properties of the materials. These results, together with other well-known physical properties, may expand future prospects for the application and study of these materials.

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