ISSN : 0974 - 7494 Volume 6 Issue 1

Trade Science Inc.

Nano Science and Nano Technology
An Indian Journal

Full Paper

NSNTAIJ, 6(1), 2012 [14-17]

Acoustic wave propagation in semiconductor ZnTe nanoparticle

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Received: 22nd December, 2011 ; Accepted: 21st January, 2012

ABSTRACT

The acoustic wave propagation in the hexagonal structured ZnTe nanoparticles has 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 ZnTe 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 other nanostructure materials and other compounds. Obtained results, together with other well known physical properties, may expand future prospects for the applications and study of this nano material.

KEYWORDS

Nanoparticle;
Elastic constants;
Longitudinal waves;
Surface waves.

INTRODUCTION

Nanometer-sized semiconductor particles belong to a state of matter in the transition region between molecules and solids. During the last three decades, research on quantum size semiconductor particles has increased enormously due to their exciting novel properties[1-4]. 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.[5]. The Formation process was discussed and it revealed a uniform hexagonal shape of ZnTe nanoparticles with good dispersion, average particle size is found to be 2.6 nm[6-9]. 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 are due to its appealing properties in electro-optical and electron acoustic devices[10-12]. Experimentally ZnTe is found to have room temperature direct bad gaps of 2.4 eV[13].

There are three types of acoustic mode lattice vibration: one longitudinal acoustic and two transverse acoustical for hexagonal and cubic structured materials[14, 15]. The one longitudinal sound velocity and one transverse sound velocity for ZnTe has been reported in[16] but all the three type of acoustic wave velocity of ZnTe are not reported in literature. Therefore in this paper, we have calculated the three types of acoustic wave velocities of ZnTe nanoparticles for each direction of propagation of wave using the second order elas-

tic constants that are important for surface and structural study of ZnTe. The calculated ultrasonic parameters are discussed with related thermophysical properties for the characterization of the chosen nanomaterial. The obtained results are interesting for the characterization of ZnTe nanoparticles.

THEORY

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

Theory for the non-linear elastic cnstants

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

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

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

Where, U is elastic energy density, $e_I=e_{ij}$ (i or j = x, y, z, I=1, …6) is component of strain tensor. Equations (1) and (2) lead six SOEC and ten TOEC for the hexagonal structure materials[17, 18].

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

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

where p = c/a: axial ratio; $C' = \chi a / p^5$; $B = \psi a^3 / p^3$; $\chi = (1/8)[\{nb_0 (n-m)\}/\{a^{n+4}\}]$ $\psi = -\chi /\{6a^2(m+n+6)\}$; m, n=integer quantity; b_0=Lennard Jones parameter.

Theory for the acoustic wave velocity

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[18]. On the basis of mode of atomic vibration, there are three types of velocities (longitudinal, quasi shear and shear) in acoustical region. The Debye average velocity (V_D) can be calculated from the initial slope of these three acoustical branches[19]. These velocities vary with the direction of propagation of wave from the unique axis of hexagonal structured crystal[20, 21].

RESULTS AND DISCUSSION

Higher order elastic constants

The unit cell parameters 'a' (basal plane parameter) and 'p' (axial ratio) for ZnTe 4.28Å and 1.637[22, 23] respectively. The value of m and n for chosen material are 6 and 7. The value of b_0 for ZnTe is 1.4×10^{-63} erg cm^7. The SOEC and TOEC have been calculated for ZnTe nanoparticle using Eq. (3) and are presented in TABLE 1.

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 second order elastic constants of ZnTe[24]. The bulk modulus (B) for ZnTe can be calculated with the formula $B= 2(C_{11}+ C_{12}+ 2C_{13} + C_{33}/2)/9$. The evaluated B for ZnTe is presented in TABLE 1. The Debye temperature Also, the comparison can be made with the value of Debye temperature ZnTe. The present Debye temperature for ZnTe is 218.4 ^{0}K, calculated using second order elastic constants. The Debye temperature experimentally determined by Lee[25] is 225.3 ^{0}K. Thus our theoretical approach for the calculation of second order elastic constants for nanostructured material at room temperature is well justified. However, third order elastic constants

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TABLE 1 : SOEC and TOEC & bulk modulus (B) in the unit of $10^{10}Nm^{-2}$ of ZnTe nanoparticle at room temperature.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B
ZnTe	8.731	2.144	1.869	9.013	2.242	3.424	4.249
ZnTe[24]	8.56	3.70	3.00	9.26	2.02	2.43	

	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{344}	C_{144}	C_{155}	C_{222}	C_{333}
ZnTe	-142.37	-22.57	-4.79	-6.09	-30.44	-28.54	-7.10	-4.73	-112.65	-114.71

are not compared due to lack of data in the literature but the negative third order elastic constants are found our previous papers for hcp structure materials[17, 18, 20, 21]. Hence applied theory for the evaluation of higher order elastic constants at room temperature is justified.

Ultrasonic velocity and allied parameters

The computed orientation dependent ultrasonic wave velocities and Debye average velocities at 300 K are shown in Figure 1. Figure 1 shows 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.

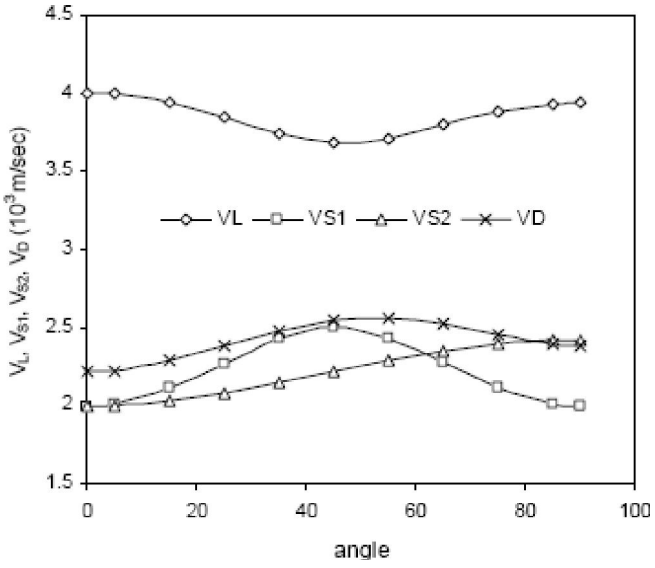

Figure 1 : V_L, V_{S1}, V_{S2}, V_D vs angle with unique axis of crystal

The nature of the angle dependent velocity curves in the present work is found similar as that for different hexagonal nano structured materials[17-21, 26]. The chosen material has shown similar properties with their crystal structure. The longitudinal and shear velocities of ZnTe are 3.99x 10^3 m/s and 2.00x 10^3 m/s respectively, while 3.59x10^3 m/s and 2.74x 10^3 m/s have evaluated by Bijalwan et al.[16]. Hence values of velocities are in good agreement with experimental/theoretical values. Thus the angle dependency of the velocities in nanostructure material is justified.

V_D of ZnTe is increasing with the angle and has maxima at 55° at 300 K (Figure 1). Since V_D is calculated using V_L, V_{S1} and V_{S2}[17, 21], 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 ZnTe is 218.4 ^{0}K. The Debye temperature experimentally determined by Lee[25] is 225.3 ^{0}K. Debye (average) sound velocity is useful for the evaluation of Debye temperature[19] and the Debye temperature is well related to specific heat per unit volume and thermal energy density[26]. The Debye average velocity for ZnTe is 2.210x10^3 m/s which have 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 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 ZnTe is 0.63. A comparison of these anisotropy values with those of GaN, AlN, InN (III group nitride-semiconductor)[27, 28] implies that the elastic anisotropy of ZnTe 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.

CONCLUSIONS

The adopted method for theoretical study of higher-order elastic constants is justified for the ZnTe nanoparticles. Although, the nature of angle dependency

of acoustical velocity in ZnTe 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 ZnTe nanoparticles.

Thus obtained results in the present work can be used for further investigations, general and industrial applications. The acoustic behavior in ZnTe 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 nanomaterials.

ACKNOWLEDGMENTS

The author wish to express sincere thanks to Dr. Ashok K. Chauhan, President, AMITY School of Engineering and Technology (ASET), New Delhi, Prof. B. P. Singh, Senior Director, Prof. (Dr.) Rekha Agarwal, Director, ASET New Delhi, Prof. S. K. Kor and Prof. Raja Ram Yadav, Department of Physics, Allahabad University, for encouraging and providing necessary facilities in carrying out the work.

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