Debye Temperature and the Structure of Nanocrystalline materials

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Abstract: **The Debye model is used for deriving many thermodynamical and electrical properties of materials. In this work, Debye model is introduced in the calculation of lattice constants from the elastic constants.**
The mean acoustic velocity in these materials is calculated from the frequency of vibrating phonons. The ultrasonic velocity is calculated from the available elastic constants of GaAs, AlAs, InP and InAs having cubic structure. The acoustic velocities are compared and the correlation with the Debye model is used to calculate the lattice constants of the materials mentioned above. The percentage error of the lattice constants being around 2%, shows the good agreement of the structure calculation of these materials.

Keywords: Ultrasonic velocity, Debye model, phonon vibration, Lattice constant.

I. INTRODUCTION

Debye model was developed for heat capacity of solids as early as 1912 by Peter Debye. Here the Debye model is used to find the lattice constant for isotropic structures. In this work, ultrasonic velocities are derived from the elastic constants. This acoustic velocity is then correlated with the Debye model to calculate the Debye temperature. Wherefrom the lattice constants are found for isotropic nanocrystalline structures, GaAs, AlAs, InP and InAs having cubic structure. The lattice constants are in good agreement with the theoretical data. Debye temperatures and Debye models were being used to calculate the structures and characteristics of materials[1]-[5].

II. THEORY

The Debye temperature from the Debye model is related to stiffness of the bonds between atoms, velocity of sound in materials and density of the material from the relation

$$\theta_D = \frac{hv}{k}\left[\frac{6\pi^2 N}{V}\right]^{1/3} \quad (1)$$

where, v is sound velocity, (N/V) is the density. Also Debye temperature is given by

$$\theta_D = \frac{h}{k}\left(\frac{9N_A}{4\pi V}\right)^{1/3}\left[\frac{2}{u_L^3}+\frac{1}{u_t^3}\right]^{-1/3} \quad (2)$$

where, h is the Planck's constant, K is the Boltzmann's constant, N_A is the Avogadro number, V is the Molar volume, u_t is the Longitudinal velocity and u_L is the Transverse velocity.
Longitudinal velocity is the axial velocity. It is found using Young's Modulus and the density, as,

$$u_t = E/\rho \quad (3)$$

Transverse velocity (u_L) is found from the formula as,

$$u_L = \left(K + \frac{4}{3}G\right)^{1/2}\rho^{-1/2} \quad (4)$$

the shear modulus (G) and the Bulk modulus (K) can be calculated using the formula,

$$K = \frac{E}{3(1-2v)} \quad (5)$$

$$G = \frac{E}{2(1+v)} \quad (6)$$

OR

$$K = (C_{11} + C_{12})/3 \quad (7)$$

$$G = (C_{11} + C_{12})/2 \quad (8)$$

Elastic Stiffness Constants are the constants of proportionality between the components of stress and strain. They are therefore related to the elastic moduli. For cubic crystals like GaAs, AlAs, InAs and InP with zinc blende structure the coefficients are C_{11}, C_{12}, C_{44} [2].

$$\lambda = C_{12} \quad (9)$$

$$\mu = (c_{11} - c_{12}) / 2 \quad (10)$$

where λ and μ Lame's constants which can be expressed as,

$$\lambda = Ev / (1 + v)(1 - 2v) \quad (11)$$

$$\mu = E / 2(1 + v) \quad (12)$$

In a solid, the lattice vibrations are quantized by phonons. By quantum mechanical approach, the phonon can be visualized to be a particle in a box of length, L. The minimum wavelength of the phonon vibration is given as

$$\lambda_n = \frac{2L}{n} \quad (13)$$

where n is a positive integer. The frequency of the vibrating phonons can be determined from the speed of sound inside the solid.

$$v_n = \frac{v_m}{\lambda_n} = \frac{nv_m}{2L} \quad (14)$$

Where v_m represents the mean acoustic velocity calculated from the longitudinal and transverse velocities as

$$v_m = \left[\frac{2}{u_L^3} + \frac{1}{u_t^3}\right]^{-1/3} \quad (15)$$

The Debye temperature is the temperature at which the wavelength of vibration of the atoms in a crystal lattice is equal to the length of the unit cell. The Debye frequency occurs when the wavelength of the phonon frequency reaches the size of the smallest unit of the lattice which is the length of the unit cell. The Debye cut off frequency or temperature separates the collective thermal lattice vibration from the independent thermal lattice vibration. This sets the constraint for the minimum wavelength of the vibration[1]. Hence,

$$a = \lambda_{min} \quad (16)$$

This minimum wavelength can be arrived in terms of the Debye temperature as

$$\lambda_{min} = \frac{hv_m}{k_B \theta_D} \quad (17)$$

III. RESULTS

The Youngs modulus, density and Poissons ratio of GaAs, AlAs, InAs and InP were taken from the literature [6] which is given in table 1.

Material	*P (kg/m^3)*	E (GPa)	*v*
GaAs	**5318**	**85.9**	**0.31**
AlAs	**3598**	**83.5**	**0.32**
InAs	**5667**	**51.4**	**0.35**
InP	**4810**	**61.1**	**0.36**

Table 1 – Material data from literature

Further, the Bulk modulus, the Shear Modulus and the Mean Velocity were calculated using equations (7), (8), (14) which are given in table 2.

Material	K (GPa)	G (GPa)	u_M (m/s)
GaAs	**75.3**	**32.79**	**2856.26**
AlAs	**77.31**	**31.63**	**3436.54**
InAs	**57.11**	**19.03**	**2268.85**
InP	**72.7**	**22.46**	**2583.10**

Table 2 – Elastic constants calculated from the empirical formula

The bulk modulus of the nanocrystalline materials and the mean velocity are shown in figure 1 and figure 2 respectively.

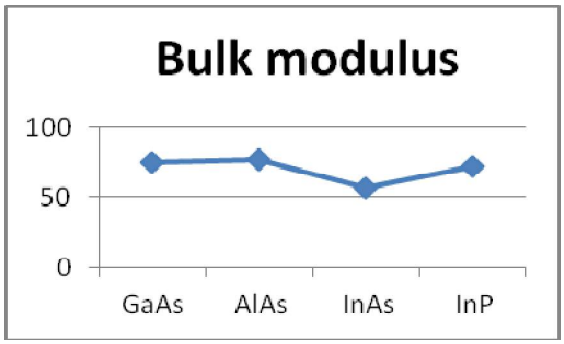

Figure 1 - Bulk modulus, (K), (in random order).

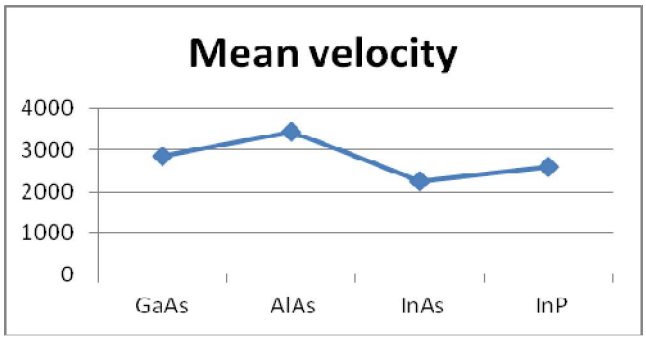

Figure 2 - The mean velocity (u_M) of the zinc blende structure compounds.

The Debye temperature as said earlier can be calculated using various physical parameters such as Young's modulus, Shear modulus and Bulk modulus which are all elastic moduli. An elastic modulus, measures an object or substance's resistance to being deformed elastically when a force is applied to it. The lattice constant is the physical dimension of unit cells in a crystal lattice.

As the Debye temperature of elements are calculated the Debye temperature of compounds of zinc blende structure can also be calculated. Table 3 gives both the calculated and the existing values of Debye temperatures

Material	Θ_D (K) (Calculated)	Θ_D (K) (Actual)	Error (%)
GaAs	**353.85**	**360**	**1.7**
AlAs	**421.9**	**417**	**1.2**
InAs	**285.28**	**280**	**1.9**
InP	**316.30**	**321**	**1.5**

Table 3 – Debye temparetures of the nanocystalline materials

Figure 3 shows the graph shows the θ_D (calculated) and θ_D (actual) in decreasing order of value. The graph depicts that the error in the values of the calculated and theoretical values of the Debye temperature is less than 2%

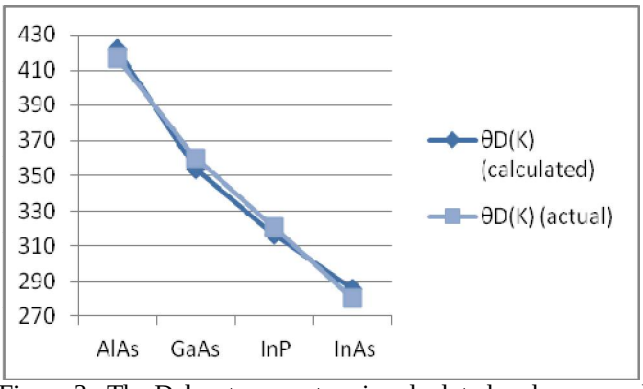

Figure 3 - The Debye temperature is calculated and compared with the theoretical Debye temperature values.

The Lattice constant being the minimum phonon vibration wavelength was calculated using the equation (17). The calculated values are compared and shown in table 4, with the percentage errors. This result is also depicted as graph in figure 4.

Material	Lattice constant (A^o) (Calculated)	Lattice constant (A^o) (Actual)	Error (%)
GaAs	**5.74**	**5.65**	**1.6**
AlAs	**5.82**	**5.66**	**2.8**
InAs	**6.15**	**6.05**	**1.6**
InP	**5.95**	**5.86**	**1.5**

Table 4 – The calculated Lattice constant shown with error percentage

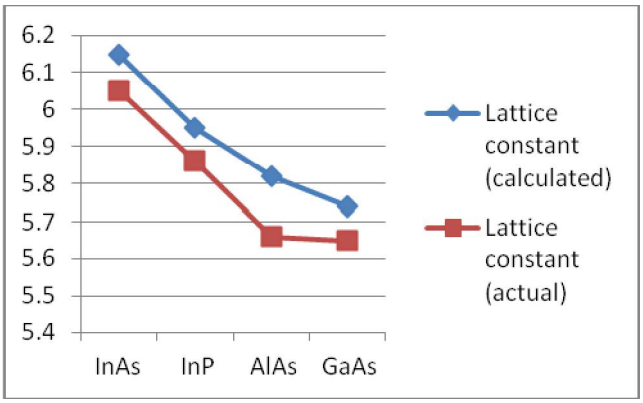

Figure 3 - The calculated and actual lattice constants comparison

Figure 3 shows the Lattice constant(calculated) and Lattice constant(actual) in decreasing order of value. It is inferred that the error between the calculated and theoretical values is less than 3%.

IV. CONCLUSIONS

The calculated Debye temperature and Lattice constant are in agreement with their theoretical values. The Bulk modulus, Shear modulus and the Mean velocity are also calculated by using similar parameters used in calculating Debye temperature and Lattice constant. In the calculations the error incurred did not exceed beyond 3% of the theoretical values. This indicates that the Debye model is also a tool to calculate the lattice constants of isotropic structured materials.

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