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Semiconductor physics

Empirical prediction of thermal properties, microhardness and sound velocity of cubic zinc-blende AlN

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Abstract. Based on some empirical formulas and some data reported in the literature, this contribution aims to study the correlation between several physical properties of cubic zinc-blende aluminium nitride (c-AlN) semiconducting material. So, we report an empirical prediction at room temperature of the Debye temperature, Debye frequency, melting temperature, thermal conductivity, Vickers hardness, and sound velocity of c-AlN. Our calculated results are compared with other data of the literature; they are in very good agreement with other data previously published. At room temperature, the Debye temperature was found at around 978.84 K, the thermal conductivity is 3.82 $W \cdot cm^{-1} \cdot K^{-1}$, while the melting temperature is around 2967.4 K, respectively. The deviations of the Debye temperature and melting temperature between our obtained values and the theoretical ones of the literature are less than 0.92% and 1.1%, respectively. Our findings on the different quantities of the zinc-blende phase have been compared to those of the hexagonal wurtzite phase. In general, no significant differences in the different quantities values between zinc-blende and wurtzite phases of AlN compound have been observed.

Keywords: thermal properties, microhardness, sound velocity, aluminium nitride.

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1. Introduction

Recently, III-V semiconducting compounds have attracted increasing interest because of its several advantages; they are technologically important materials for numerous electronic and optoelectronic applications such as short-wave light emitting diodes, optical detectors, and high-frequency optoelectronic devices [1, 2]. Among these compounds, the aluminium nitride (AlN) that has the wurtzite (B4) structure under normal conditions [3, 4]. Sahoo [5] investigated the effect of piezoelectric polarization on phonon group velocity of III-nitride (GaN, AlN, and InN) semiconducting compounds in B4 phase. They found that the effect of piezoelectric polarization on phonon group velocity does not exceed 1% in all the studied materials.

The structural parameters, elastic constants and some other physical properties of wurtzite and zinc-blende (B3) phases of AlN material have been studied experimentally [6] and theoretically [7-10]. Under hydrostatic pressure, it was found that AlN exhibits first-order phase transition from its initial zinc-blende-type structure to the rock-salt-type structure at the pressure 19.6 GPa [11]. Sarwan and Singh [12] investigated the pressure induced crystal properties of group III-nitrides by means of modified interaction potential model (MIPM). They found that the cubic zinc-blende phase of AlN transforms to the cubic rock-salt phase at the pressure around 21 GPa [12]. Using the molecular dynamics simulation method, Goumri-Said *et al.* [13] studied the structural and thermodynamic properties of the zinc-blende AlN material. As first-principle calculations provide the most reliable information on atomic-scale materials properties, Ramírez-Montes *et al.* [14] used these calculations to study the increasing yttrium fraction on structural, thermodynamic and optoelectronic properties of $Y_xAl_{1-x}N$ semiconducting alloys in both rock-salt and wurtzite phases. Using the *ab initio* pseudopotential method based on the density-functional theory (DFT), Saib and Bouarissa [15] investigated the electronic properties and elastic constants of AlN in the wurtzite, zinc-blende and rock-salt structures. Using the first principles according to density function theory, Yang *et al.* [16] have studied the structural, elastic, thermodynamic, electronic and optical properties of several predicted novel phases of AlN

material. Although several physical properties of AlN semiconducting compound were established in some other works [17, 18], only limited theoretical investigation [19] has been reported for its thermal conductivity.

In this work, a semi-empirical method was applied to investigate some thermal properties, microhardness and sound velocity of cubic zinc-blende AlN compound.

2. Theoretical, results and discussion

2.1. Debye temperature, thermal conductivity, and melting temperature

The Debye temperature θ_D is a fundamental thermo-dynamical quantity used to describe various physical properties of solids that are related to lattice vibrations [20]. It is well known that the Debye temperature correlates with many other physical properties of materials, namely: elastic constants, specific heat, and melting temperature [20, 21]. To relate the Debye temperature θ_D with other physical parameters of solids, Kumar *et al.* [22] proposed a linear relationship between the Debye temperature θ_D and the plasmon energy $\hbar\omega_p$, it is given by the following formula [22]:

$$\theta_D = -K_1 + K_2\left(\hbar\omega_p\right). \tag{1}$$

The values of the constants K_1 and K_2 for group III-V semiconducting materials are 800.88 K and 77.48 K/eV, respectively [22].

Replacing the value (22.97 eV) [23] of the plasmon energy in the previous formula, the value of θ_D has been calculated and found to be 978.84 K. Our obtained value of θ_D is slightly higher than the theoretical values 926 and 948 K reported by Yong *et al.* [21], and slightly lower than the theoretical value 998.5 K reported by Xu and Bu [24], it is in excellent agreement with the values 970 and 964.18 K reported by Marmalyuk *et al.* [25] and Wang [26], respectively. The deviations of θ_D between our value (978.84 K) and the values 970 and 964.18 K reported by Marmalyuk *et al.* [25] and Wang [26] are only around 0.91% and 1.52%, respectively. No significant differences in θ_D values between zinc-blende and wurtzite phases of AlN compound have been reported in the literature [24].

Another linear relationship between the Debye temperature θ_D and the quantity $\left[1/\left(M^{1/2}\cdot d^{5/4}\right)\right]$ has been established, it is expressed as follows [27]

$$\theta_D = K_3\left[1/\left(M^{1/2}\cdot d^{5/4}\right)\right] - K_4, \tag{2}$$

where M is the mean atomic weight, d – bond length, and K_3 and K_4 are two empirical parameters slightly depending on the nature group of material. The values of the constants K_3 and K_4 for group III-V semiconducting materials are $K_3 = 112.66\cdot10^{-12}$ $Kg^{1/2}\cdot m^{5/4}\cdot K$ and $K_4 =$ = 90.74 K, respectively [27]. Replacing the value ($1.8966\cdot10^{-10}$ m) deduced from the lattice parameter (4.38 Å) [6] of the bond length in the previous formula, the value of θ_D has been calculated and found to be 1027.38 K. This value is slightly higher than the theoretical ones 926 and 948 K reported by Yong *et al.* [21], it is in general in agreement with the value 998.5 K reported in Ref. [24]. The deviation of θ_D between our value (1027.38 K) and the value 998.5 K reported by Xu and Bu [24] is close to 2.9%.

The Debye frequency f_D plays an importance role in the heat transport in a lattice; it is defined as the maximum vibrational frequency of a given mode in a crystal [28]. For an acoustic phonon branch, the maximum frequency f_D and the acoustic Debye temperature θ_a are related by [28]

$$f_D = \frac{k_B}{h}\theta_a, \tag{3}$$

where $k_B = 1.38062\cdot10^{-23}$ $J\cdot K^{-1}$ is the Boltzmann constant, and $h = 6.62617\cdot10^{-34}$ J·s is the Planck constant.

The acoustic Debye temperature θ_a can be determined from the traditional Debye temperature θ_D as follows [28]:

$$\theta_a = \theta_D\cdot n^{-1/3}, \tag{4}$$

where n is the number of atoms per unit cell (the families of crystals with $n = 2$ include the rock-salt, diamond, and zinc-blende structure compounds) [28]. From Eqs. (3) and (4), we can deduce the following relationship [29]:

$$f_D \approx 16.5374\cdot10^9\,\theta_D, \tag{5}$$

where f_D is expressed in Hz and θ_D is expressed in K.

Replacing in Eq. (5) the Debye temperature θ_D (978.84 K) obtained in this work, the value of the Debye frequency f_D of the zinc-blende AlN compound has been calculated and found to be close to 16.2 THz. Our obtained value of f_D is slightly lower than the theoretical one 20.81 THz reported by Xu and Bu [24].

Another important thermal parameter of material is the thermal conductivity. Heat energy in a solid can be carried by two fundamental mechanisms. The first one: electronic carriers (electrons and holes) that are the most dominant in metals; second one: lattice waves (phonons) that are the most dominant in semiconductor and insulator materials. Lattice defects or imperfections, electromagnetic and spin waves in ferromagnetic and anti-ferromagnetic materials as well as some other excitations can also affect considerably the thermal conduction processes in the solid. In the case of isotropic material; the heat conduction is defined by Fourier's law [30]:

$$Q = \kappa\nabla T, \tag{6}$$

where Q is the heat flux, ∇T – temperature gradient, and κ – scalar thermal conductivity. The isotropic scalar

equation form is usually applicable to many structures, such as: cubic crystal solids, polycrystalline materials and also amorphous solids [30]. The thermal conductivity κ of wide-band gap group IV and group III-V semiconductors is discussed by Morelli and Slack [28], and a performant model for the magnitude of the thermal conductivity at temperatures near the Debye temperature is presented as follows [28]:

$$\kappa = A\frac{\overline{M}\,\theta_D^3\,\delta}{\gamma^2 T n^{2/3}}, \tag{7}$$

where $A = \frac{2.43\cdot 10^{-8}}{1-0.514/\gamma+0.228/\gamma^2}$, $\overline{M}$ is the average atomic mass, θ_D – traditional high-temperature Debye temperature, δ^3 – volume per atom, γ – high temperature Grüneisen constant, T – temperature, and n – number of atoms per unit cell.

Replacing in Eq. (7) the experimental lattice parameter (4.38 Å) [6] obtained at room temperature, our theoretical value (978.84 K) of the Debye temperature θ_D, and the theoretical Grüneisen constant γ (0.89) [31], the value of κ of the zinc-blende AlN compound has been calculated and found to be 3.82 $W\cdot m^{-1}\cdot K^{-1}$. Our obtained value of κ is very higher than the theoretical one 1.86 $W\cdot m^{-1}\cdot K^{-1}$ reported in our previous work [19]. Although no direct comparison is possible with experimental or another theoretical predictions due to a lack of data (except the value 1.86 $W\cdot m^{-1}\cdot K^{-1}$ [19]) in the literature on the thermal conductivity κ of the zinc-blende phase, our value is slightly higher than the experimental value (3.5 $W\cdot m^{-1}\cdot K^{-1}$) reported by Morelli and Slack [28] for the hexagonal phase (w-AlN). It can be noted that our result is in agreement with the Morelli–Slack theory and the results reported by AlShaikhi and Srivastava [32], which predicts that the thermal conductivity of the cubic zinc-blende phase AlN is higher than that of the hexagonal phase. It is very important to note that the Morelli–Slack theory was also verified very recently for gallium pnictides GaX (X = P, As, Sb) semiconducting materials [33]. It was found that the values of the lattice thermal conductivity of the zinc-blende phase GaX (X = P, As, Sb) semiconducting materials are slightly higher than those of the hexagonal wurtzite phase.

Adachi [31] proposed a linear relationship between the melting temperature T_m and lattice parameter for some group IV, III-V and II-VI semiconducting materials with cubic and hexagonal structures. This linear relationship is given by the following formula [31]

$$T_m = 7159 - 957a, \tag{8}$$

where a is expressed in Å and T_m is expressed in K.

Replacing in Eq. (8), the lattice parameter (4.38 Å) [6] obtained at room temperature, the value of T_m of AlN compound with the zinc-blende structure has been calculated and found to be 2967.4 K. This value agrees very well with the theoretical values 3000 K and 3060 K reported by Yaddanapudi [18] and in our previous work [19], respectively. The deviation of T_m between our value (2967.4 K) and the theoretical one (3000 K) reported by Yaddanapudi [18] is only about 1.1%. Since both polytypes (zinc-blende and wurtzite) have the same tetrahedral bonding (negligible difference in their chemical bonding) [34], our value of T_m agrees also well with the experimental values of 3025 K [35] and 3023 K [36] of the hexagonal w-AlN compound. No significant difference in the T_m values between zinc-blende and hexagonal phases of GaN and ZnS binary semiconductors has been reported in the literature [31]. We hope that the present result on T_m is a reliable estimation for AlN compound with zinc-blende structure.

For groups III-V and II-VI semiconducting materials, Kumar *et al.* [22] proposed another linear relationship between the melting temperature T_m and plasmon energy ($\hbar\omega_p$), it is given by the following formula:

$$T_m = -K_5 + K_6(\hbar\omega_p). \tag{9}$$

For group III-V semiconducting compounds, the values of the constants K_5 and K_6 are 1604.02 K and 204.7 K/eV, respectively [22]. Replacing the value (22.97 eV) [23] of the plasmon energy in Eq. (9), the value of T_m has been calculated and found to be 3097.94 K. This value is in good agreement with the theoretical value 3060 K reported in our previous work [19]. The deviation of T_m between our value (3097.94 K) and the theoretical one (3060 K) reported in our previous work [19] is only around 1.24%.

2.2. Vickers hardness

One of important mechanical properties of solid is its hardness; it is usually taken to be a measure of the resistance of a solid to local plastic deformation [37]. Bulk modulus or shear modulus can measure the hardness [12]. In order to determine the hardness of cubic zinc-blende AlN material, two empirical formulas were applied. The Vickers hardness H_V and shear modulus G are related by the following empirical formula [38]

$$H_V = 0.1475G. \tag{10}$$

Second empirical formula related the Vickers hardness H_V and the isotropic shear modulus G is given as follows [38]

$$H_V = 0.1769G - 2.899. \tag{11}$$

Replacing the value (123.47 GPa) [19] of the isotropic shear modulus G in Eqs. (10) and (11), the values of the Vickers hardness H_V of our material of interest have been calculated and found to be 18.21 and 18.94 GPa, respectively. Our obtained values regarding the Vickers hardness H_V are slightly lower than the theoretical values 20.043 and 25.4 GPa, reported by Xu

and Bu [24], and Bahadur and Mishra [39], respectively, and slightly higher than the value 16.9 GPa reported by Yang *et al.* [16], they are in excellent agreement with the experimental result (18 GPa) of the wurtzite phase [40, 41], and the theoretical value of 18.42 GPa reported recently by Zagorac *et al.* [42]. The discrepancy between our value 18.21 GPa and the experimental one (18 GPa) of the wurtzite phase [40, 41] is less than 1.17%, while the deviation between our value 18.21 GPa and the theoretical one 18.42 GPa [42] is only around 1.14%. No significant differences in the hardness values between zinc-blende and hexagonal (wurtzite) phases of AlN, AlP, and AlAs semiconducting compounds have been reported in the literature [24].

2.3. Sound velocity

Acoustic waves are the mechanical waves that cannot propagate through vacuum; they can pass through a solid, liquid or gas. When these waves pass through a solid they are known as elastic waves, while when they pass through liquid or gas, they are known as acoustic waves [20]. The knowledge of the sound velocity can play in important role in material science. It can be help on the determination of several properties such as the thermal conductivity and acoustic Grüneisen parameter. Experimentally, the elastic stiffness constants of crystal can be also determined from the measurement of the sound velocity for longitudinal and transverse acoustic waves in different crystallographic directions [43]. In the Debye model, the sound velocity V_S and the Debye temperature θ_D are related by the following expression [43]:

$$V_S = k_B \theta_D \Big/ \sqrt[3]{6\pi^2 \hbar^3 N/V} \,, \qquad (12)$$

where N/V represents the concentration of atoms in solid.

Replacing in Eq. (12) our value (978.84 K) of the Debye temperature θ_D, one can obtained the value V_S for AlN compound close to 7203.2 m/s. Our obtained value (7203.2 m/s) of V_S is slightly higher than the theoretical value (6805.4 m/s) reported in our previous work [19], and the values 6859 and 6833 m/s reported by Yong *et al.* [21]. Our value of V_S is slightly lower than the theoretical value (7500 m/s) reported by AlShaikhi and Srivastava [32]. So, it is localized between the different theoretical values of the literature.

3. Conclusions

In summary, using some empirical formulas and some data of the literature, we calculated some physical properties of zinc-blende AlN semiconducting material.

Parameters such as the Debye temperature, Debye frequency, melting temperature, thermal conductivity, Vickers hardness, and sound velocity have been predicted. The values obtained are in good agreement with other theoretical results of the literature.

The Debye temperature θ_D and the melting one T_m have been found as 978.84 K and 2967.4 K, respectively. The deviations of θ_D and T_m between our values and the theoretical ones 970 K and 3000 K of the literature are less than 0.92% and 1.1%, respectively. The zinc-blende AlN has been found to be the very efficient heat conductor with a room temperature thermal conductivity of around 382 $W \cdot m^{-1} \cdot K^{-1}$. Our value 7203.2 m/s of the sound velocity V_S has been found to be localized between the different theoretical data of the literature.

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