Structural properties and temperature dependence of phase transition point of zinc blende clusters: BN, BP, AlN, and AlP

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Abstract

Ab initio calculation with restricted Hartree-Fock method (RHF) for eight-atom zinc blende lattices (BN, BP, AlN, and AlP) has been used to study the structural properties and the behavior of the phase transition with increasing pressure and temperature. A simple empirical equation is suggested to illustrate this behavior, and also a new parameter, the variation rate (ζ), is used to simplify the results. It is found that this rate decreases with temperature. The prominent drawback of this paper is the lack of experimental data for comparison.

Keywords: Structural properties, temperature, phase transition, III-V materials.

Introduction.

The nano sized field is a promising trend to get better, unique materials,[1] and high performance devices,[2,3] via the dependence of these nano-structures' properties upon the size.[4,5] In this respect, III-V nano semiconductors seem to be among the most interesting type of materials due to their impressive characteristics and applications.[6] On the other hand, many researchers have studied materials on almost the size of lattice,[7-10] however most of them have investigated the properties of nano sized materials either a alone or under a variable.[11-18] So the aim of the present work is to investigate the structural properties and the simultaneous effect of pressure and temperature on the phase transition behavior of some III-V semiconductors in the nano scale using restricted Hartree-Fock method (RHF). The calculations are accomplished by means of the *GAUSSIAN 03* program.[19]

Assumption

The kernel of this proposal is the lattice volume at which a phase transition (PT) occurs. When PT's pressure is applied the volume will reach a limit that turned it into another phase, however, the same volume will be changed due to the temperature, so a specific pressure needs to be exerted to get the initial limit of the volume at which the phase transition initiates. **Figure 1** shows our assumption clearly:

Calculations

Table 1 shows our calculated properties for the four materials.
After the determination of PT's pressure at zero temperature (P_t),[36]

$$P_t = 0.1[\frac{B_o}{20-\lambda}]^3 \tag{1}$$

Where λ is a constant (= 1, 5 and 8 for IV, III-V and II-V groups respectively).[36]
We calculated the volume at this pressure[37]:

$$V = V_o[1 + P\frac{B_o'}{B_o}]^{-\frac{1}{B_o'}} \tag{2}$$

Then both of them were fixed. Next, the change of lattice constant with temperature has been calculated from[38]

$$\alpha = \frac{1}{a_o}\frac{da}{dT} \tag{3}$$

Where α is the linear thermal expansion,[38] V_o and B_o are the volume and the bulk modulus at the fixed conditions of pressure-temperature (0, 0), P is the pressure, V and a are the volume and the lattice constant of the unit cell at any temperature T respectively,[39] and B'_o is the derivative of bulk modulus at zero pressure and it is calculated from Eq.(4).[40]

$$B'_o = 1 + \frac{2.3}{3}\frac{r_{wse}}{l} \qquad (4)$$

Here l is the length scale and r_{wse} is the radius at the equilibrium [40]. According to Omer (αT_m=0.021),[41] T_m represents the melting temperature (= 3000, 2800,[42] 2500,[43] and 2100,[42] for BN, BP, AlN, and AlP respectively), then Eq.(3) will be,

$$a = a_o(1 + 0.021\frac{T}{T_m}) \qquad \text{or} \qquad (5)$$

$$a = a_o X$$

where

$$X \equiv (1 + 0.021\frac{T}{T_m}) \qquad (6)$$

According to Cohen empirical equation for III-V zinc-blende materials which is:[44]

$$B = \frac{1970 - 200I}{d^{3.5}} \qquad \text{or} \qquad (7)$$

$$= const. \times d^{-3.5}$$

Where (d) is the bond length, and it equals for zinc blende materials (= 0.433 a), and I is the ionicity factor (= 0, 1 and 2 for IV, III-V and II-V groups respectively).[44] By gathering this result with Eq.(5) one can get:

$$d = 0.433a_o X \qquad \text{or} \qquad (8)$$

$$= d_o X$$

By combining Eq.(8) and Eq.(7):

$$B = B_o X^{-3.5} \qquad (9)$$

We have from Eq.(2) and Eq.(5):

$$\frac{V}{V_o} = X^3 = [1 + P_T\frac{B'_o}{B}]^{-\frac{1}{B'_o}} \qquad (10)$$

By substituting Eq.(9) in Eq.(10) we get the pressure of phase transition at any temperature P_T:

$$P_T = \frac{B_o}{B'_o}X^{-3.5}[X^{-3B'_o} - 1] \qquad (11)$$

In general a relation between the total phase transition pressure P_{tot} and the temperature suggested for III-V ZB-materials is:

$$P_{tot} = P_t + P_T \qquad\qquad (12)$$

In order to get a better view, a variation rate has been suggested (ζ) as:

$$\varsigma = \frac{X}{P_T}; \quad \text{(GPa)}^{-1} \qquad\qquad (13)$$

We can define ζ as the relative change of temperature attributed to the pressure variation.

Results and discussion

As illustrated in **Figure 2**, the phase transition pressure increases with temperature, since the increase in temperature leads to an increase in volume of the lattice and that entails more pressure to retain the volume at the critical limit.[45]

The variation rate decreases with temperature and pressure, as shown in **Figure 3**. Here we have two parameters; compression and temperature; they will be discussed separately in order to get a complete view of their effects upon the matter:

- Compression: when it increases the distance between atoms decreases[46] and so the compressibility, while the bulk modulus increases[47] due to its dependence on the bond length.[48] According to that the resistance to deformation increases.[49]
- Temperature: its increment leads to an increment of volume and kinetic energy[50] which makes the bond weaker[51] and the bulk modulus less.[52]

According to what mentioned above the results of compression represent anti-compression factors, i.e. the more compression, the more resistance of mater. On the other hand, the effects of temperature are opposite to the effects of compression.

Acknowledgments

Conclusions

The higher the temperature, the higher the pressure for phase transition is needed, so at low temperature and high pressure a change into another phase may happen or cause a fracture, whereas the variation rate decreases with the extremely values of the exerted conditions and its slope refers to the resistance of the matter to change; this resistance is low at the beginning and high at the end. Additionally, a threshold limit appears, next to this limit the distortion almost behaves in ascending way.

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Table 1. Structural properties of BN, BP, AlN, and AlP.

Mat.	Property	Pres.	Exp.	Other		
BN	a (A)	3.748	3.615[a]	3.625[d]	3.613[f]	3.596[g]
	B_o (GPa)	325.43	369[a]	364.3[d]	386[f]	395[g]
	B_o'	3.156	4[a]	4.8[d]		3.65[g]
	$-E_c$ (eV)	5.7086	13.2[b]	12.38[e]	17.39[f]	12.94[g]
	P_t (GPa)	1021.1718	394[c]			
BP	a (A)	4.601	4.537[h]	4.459[d]	4.554, 4.543[i]	4.478[l]
	B_o (GPa)	158.7781	173[h]	164.6[d]	175, 173, 152[i]	173.4[l]
	B_o'	2.422	4.3[i]	4.7[d]	3.51[i]	3.712[l]
	$-E_c$ (eV)	11.824	10.24[j]	9.360[e]		
	P_t (GPa)	118.5894	>110[k]			
AlN	a (A)	4.359	4.37[m]	4.4[f]	4.323[l]	4.36[n]
	B_o (GPa)	191.8236	207.9[f]	198[f]	203.2[l]	
	B_o'	2.344			4.028[l]	
	$-E_c$ (eV)	13.595	11.52[f]	14.81[f]		
	P_t (GPa)	209.1377		19.69[o]		
AlP	a (A)	5.328	5.47[b]	5.45[d]	5.417[l]	5.467[n]
	B_o (GPa)	95.0126	86[b]	86.2[d]	88.6[l]	
	B_o'	2.194		4.6[d]	4.037[l]	
	$-E_c$ (eV)	15.601	8.34[b]	7.945[e]		
	P_t (GPa)	25.4138	14.2, <42[k]	170, 140, 93[p]		

a. 20.   e. 24.   i. 28.   m. 32.
b. 21.   f. 25.   j. 29.   n. 33.
c. 22.   g. 26.   k. 30.   o. 34.
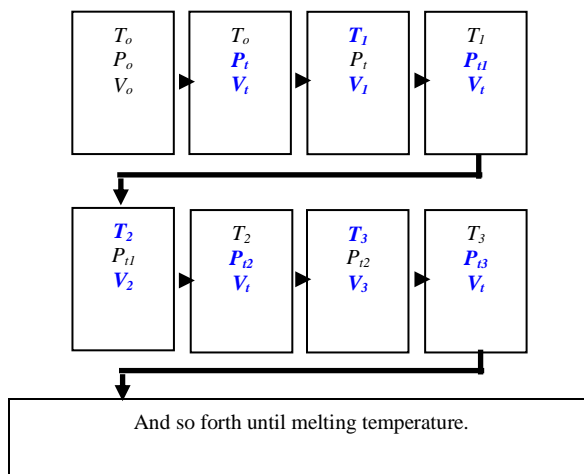d. 23.   h. 27.   l. 31.   p. 35.

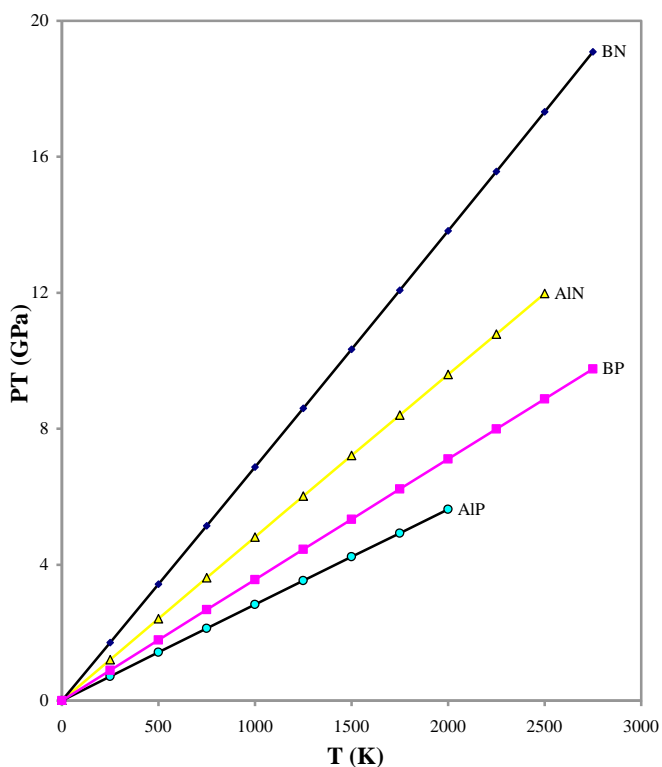**Figure (1): Steps of the assumption for phase transition volume.**

Figure (2): The change of phase transition pressure with temperature for: BN, BP, AlN, and AlP.
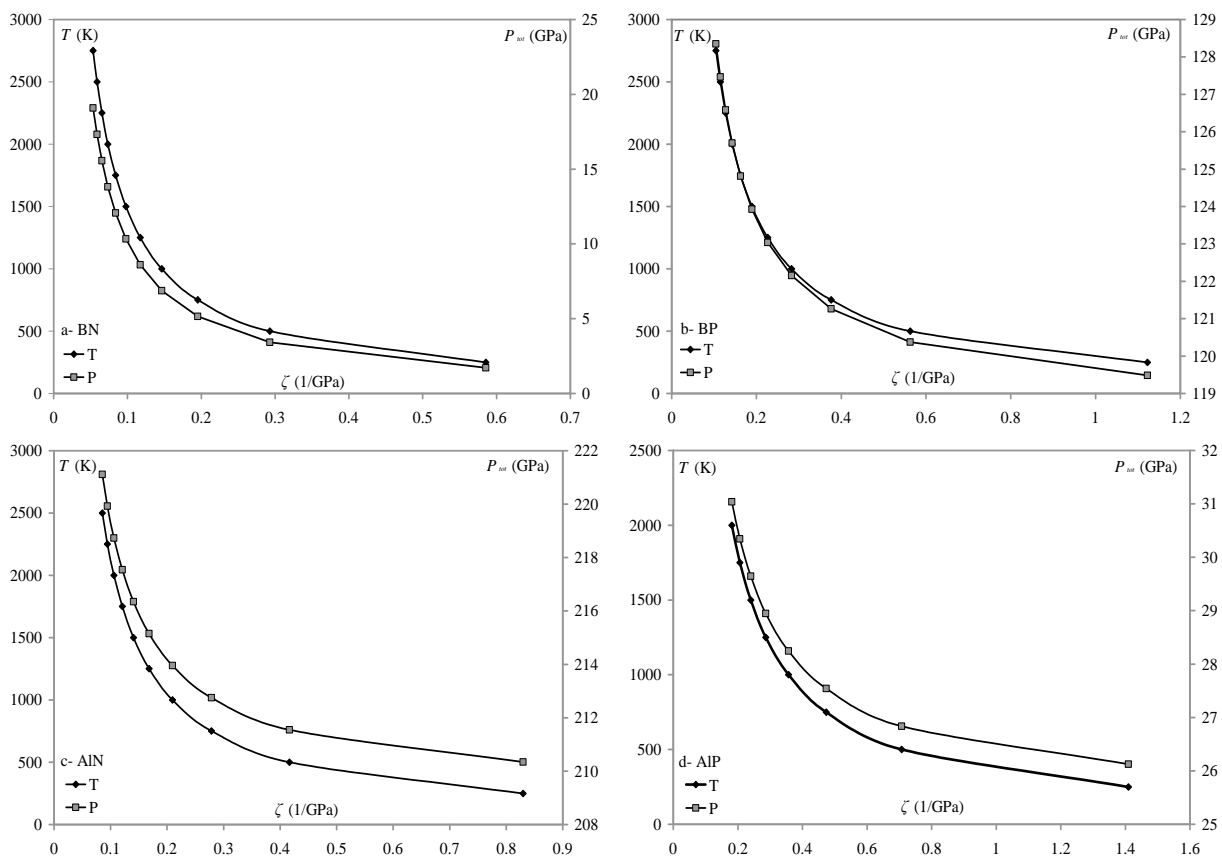
Figure (3): The change of variation rate with temperature and pressure for: BN, BP, AlN, and AlP.

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