

The Effect of Temperature on Phase Transition Pressure of Zinc-Blende Boron Nitride

Z. Y. Mijbil

Babylon University, Veterinary College.

Summary

A new semiempirical relation between the temperature (T) and the pressure of phase transition (P_t) had been presented for c-BN and III-V zinc-blende materials. The results had showed an increase in pressure of phase transition with the increase of temperature without any comparison with experimental data had been held because no other similar works about this field were found, on the other side an amorphous or a transition phase, due to the temperature, proposed to exist between the zinc-blende to rocksalt transition.

I. Introduction

The amazing aspects [Zunger and Freeman 1978] of sp^3 [Märliid 2001] cubic boron nitride (c-BN) [Jayawardane *et al.* 2001 and Yin *et al.* 2001] such as high value of hardness [Wentzcovitch *et al.* 1986], melting point [Sun *et al.* 2001], thermal conductivity [Kádas *et al.* 2000], and band gap [Mattesini and Matar 2001], and low electric conductivity [Lambrecht and Segall 1989] had made it the choice number one in many uses [Meng *et al.* 2004] as a polish, cut [Horiuchi *et al.* 1998], and shell material [Huang and Zhu 2002].

Phase transition is an important character in both industry field [Bunk *et al.* 1999] and scientific research [Lukashev and Lambrecht 2004], and as long as the c-BN is the stable form at (0 K) [Ooi *et al.* 2006] but not the steady state at the ambient conditions [Mujica *et al.* 2003] and it may transform to rocksalt (RS) structure [Sekkal *et al.* 1998], this paper has been presented in order to study the effect of temperature on the transition state under high pressure specially when we know that this substance is used for difficult jobs [Tomaszkiewicz 2002], and many other binary (ZB) zinc-blende materials behave just like c-BN [Lukashev and Lambrecht 2004, Jaffe *et al.* 1993, Spain *et al.* 1984]

II. Calculation

The general semiempirical complete neglect of differential overlap method (CNDO) with tight binding approximation (TB) is used for determining the lattice constant (a_o) and the bulk modulus at zero pressure-temperature point (B_o), the results were showed in table (1).

First the volume at the predicted pressure of phase transition ($P_t=394$ GPa) [Sekkal *et al.* 1998] was calculated from equation (1) [Tang *et al.* 2001] then both of them were fixed.

$$V = V_o \left[1 + P \frac{B'_o}{B_o} \right]^{-\frac{1}{B'_o}} \quad (1)$$

Next, the change of lattice constant with temperature had been calculated from equation (2).

$$\alpha = \frac{1}{a} \frac{da}{dT} \quad (2)$$

Where α is the linear thermal expansion (6.999×10^{-6}) [Kumar and Sastry 2001], V_o and B_o are the volume and the bulk modulus at the fixed conditions of pressure-temperature (0,0), P the pressure, B'_o the derivative of bulk modulus at zero pressure and it is constant ($B'_o = 4$) and V is the volume of unit cell and a is the lattice constant at any temperature (T).

The change in pressure that come from the volume deviation after heating is calculated from Murnagham equation of state (EOS) [Wang *et al.* 2006], at the same time the bulk modula at different temperatures with the same phase transition pressure were calculated from Cohen empirical equation for III-V zinc-blende materials which is [Zheng *et al.* 1999] as below:

$$B_o = 1772 d^{-3.5} \quad (3)$$

$$d = 0.433 a \quad (4)$$

Where d is the distance between two atoms [Wang and Ye 2002].

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

$$(5)$$

$$(6)$$

Where P_T is the pressure of transition at any temperature, B_{po} is the bulk modulus at (394 GPa, 0 K) and α is the linear thermal expansion.