THE EFFECT OF TEMPERATURE ON PHASE TRANSITION PRESSURE OF ZINC-BLENDE BORON NITRIDE

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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 had been held because no other similar works about this field were found, on the other side a transition or an amorphous phase proposed to exist between the zinc-blende to rocksalt transition.

I. Introduction

The amazing aspects [Zunger and Freeman 1978] of sp\(^3\) cubic boron nitride (c-BN) [Märlid 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 \((0 \text{ K})\) [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 for studing the effect of temperature on the transition state under high pressure specially when we know that this mater is used for difficutt jobs [Tomasziewicz 2002], and many other binary (ZB) zinc-blende materials behave just like c-BN [Lukashev and Lamberchet 2004, Jaffe et al. 1993, Spain et al. 1984].

II. Calculations

The semiempirical complete neglect of differential overlap mehtod (CNDO) with tight binding approximation (TB) is used for determining the lattice constant \((a_0)\) and the bulk modulus at zero pressure-temperature point, the results were showed in table (1).
First the volume at the predicted pressure of phase transition \( (P_t=394 \text{ GPa}) \) [Sekkal et al. 1998] was calculated from equation (1) [Tang et al. 2001], then both of them were fixed. Next, the change of lattice constant with temperature had been calculated from equation (2)

\[
V = V_o \left[ 1 + P \frac{B'_o}{B_o} \right]^{-\frac{1}{3}} \quad (1)
\]

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

Where \( \alpha \) is the linear thermal expansion \( (6.999 \times 10^{-6}) \) [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 \((=4)\), \( V \) 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:

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

\[
d = 0.433 \quad a \quad (4)
\]

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

\[
P_{tot} = P_T + P_T \quad (5)
\]

\[
P_T = \frac{B_{po}}{B_o} \left(1 - \alpha T\right)^{3.5} \left[1 - \alpha (P_T)\right]^{-3B_o} - 1 \quad (6)
\]

Where \( P_T \) is the pressure of transition at any temperature, \( B_{po} \) is the bulk modulus at \((394 \text{ GPa}, 0 \text{ K})\).
III. Results and Discussion
The result was showed in figure (1), which is a proportional relationship between temperature and pressure, and that because of the increase in temperature leads to increase in volume of the lattice [Marshed 2006] and that entails more pressure [Merdan 2005] to retain the volume at the critical limit.

IV. Conclusions
1. The long life of the c-BN structure under high pressure-temperature.
2. At high temperature c-BN needs more pressure to have phase transition.
3. At the same time at high pressure c-BN needs more temperature to melt.
4. Amorphous phase may be exist between ZB and RS transition when temperature arises and the temperature is under the limit of change.
5. The increase of temperature with phase transition pressure is assistant factor for faster phase transition process, because the proportional relation between the kinetic energy of the particles and temperature [Sibona et al. 2003] figure (2) (Note: not the total energy).
Figure (1): The effect of temperature on phase transition pressure.

Figure (2): The effect of temperature on kinetic energy.

References


