PHASE TRANSITION IN BORON NITRIDE

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ABSTRACT

The phase transition in boron nitride, interaction potential energies are calculated using a three-body interaction potential. The experimental and theoretical results are in good agreement.

Keywords: phase transition Pt, b, ρ_i f(r) are model parameters.

1. INTRODUCTION

Boron Nitride (BN) is a low porosity white solid material. It is easily machined into complex shaped using standard carbide tooling. The material is anisotropic in its electrical and mechanical properties due to the platy-hexagonal crystals and their orientation during hot press consolidation. BN can stably exist in many molyporphs because B and N atom can bind together by sp^2 and sp^3 hybridizations. BN can be found in hexagonal/ layered graphite- like phase (h-BN, r-BN), turbostratic like phase (t-BN), cubic diamond like phase (C-BN) and wurtzite like phase (w-BN) [1,2]. BN is normally found in hexagonal phase. Hexagonal BN (h-BN) is a stable phase under ambient conditions. Cubic BN and wurtzite BN are synthesized from h-BN at high temperature and high pressure [1-3].

The wurtzite W_2 phase of BN is in the metastable phase in nature. The material attracts keen interest due to its technological features such as extreme hardness, high melting point, interesting dielectric and thermal behavior. The structural, mechanical and electronic properties and the stability of BN in Pnma structure were studied using first principle calculations by Cambridge Serial Total Energy Package (CASTEP) plane wave code and the calculations were performed with the local density approximation [4]. The thermal conductivity of BN and its composites is reported elsewhere [1, 2, 5, 6]. For thermal management applications BN is found to be an electrically insulating counterpart of graphene [7, 8]. The insulating behavior of this material along with its high thermal conductivity generates a new concept for the electronic industry. Wurtzite phase of BN belongs to III group nitrides (GaN, AlN, and InN) (9-14). The structural, elastic, mechanical and acoustical properties of different phases of BN measured using X-Ray diffraction pseudo potential, DFT methods have been reported in [1,2,9-14]. Very few studies have been done in the past on the pressure- dependent elastic, structural and physical properties of boron compounds [15-17]. Therefore the present study concentrates on the elastic and ultrasonic characteristics of W-BN under the effect of pressure.Theoretical evaluation of the second order elastic constants of W-BN under the effect of pressure.

Theoretical evaluation of second order elastic constant of W-BN has been done at room temperature and at different pressure using the many- body interaction potential approach. Orientation and pressure -dependent ultrasonic velocity, thermal relaxation time and other related thermo physical parameters (Debye temperature, Debye average velocity, specific heat and thermal energy density) are also calculated using the evaluated second- order elastic constant. The obtained results are compared with the properties of other W_2 structured materials for complete analysis and characterization.

Co-workers [1-27] have studied the interaction potential energies using both two-body [1-3] and three-body [4-7] potentials. The latter potentials have given their prediction better than those revealed by other potential [1-3].Elastic

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constants are measured by Lindquist Potential [8] Singh and Verma [9] Karlsson [10]. In the present paper, we have used three-body potential to explain the phase transition, interaction potential energies of boron nitride.

Calculations have been performed using the expression for the model parameters given by Verma and co-workers [4] and those for the pressure derivatives of SOE constants are given by Garg et al [5] respectively. The essential theory and calculations are given in section 2. The results are presented and discussed in section 3.

2. THEORY AND METHOD OF CALCULATIONS:

Interaction potential energy of rock salt structure solid with contribution from the long-range coulomb and three-body interactions and the short-range repulsive and van der Waals dipole-dipole and dipole –quadrupole attractions is given by

$$W(r) = \alpha_m Z (Z+6 f(r))/r + [W_1(r)+W_2(r)] \, e^2 \qquad (1)$$

First term is the Coulomb interaction with a α_m as the Madelung constant, Ze is the ionic charge and e is the electronic charge. Here r ($=r_0$) and r_1 ($=2r_0$) are the first and second neighbor distances. $f(r)$ is the three-body force parameter dependent on r. W_1 and W_2 are the short-range interactions defined as

$$W_1(r) = b\beta/e^2\beta_{+-} \exp(r_+ + r_- -r)/\rho_{+-} \, -C_{+-}/r^6 - d_{+-}/r^8 \qquad (2)$$

$$W_2(r') = b\beta/e^2 \, \beta_{++}\exp (2r_+ + r')/\rho_{++} + b\beta_{--}/e^2\exp (2r_- - r')/\rho_{--} \, -(c_{++} +c_{--})/r'^6 \, -(d_{++} +d_{--})/r'^8 \qquad (3)$$

$$\text{Where } \beta_{ij} = 1+ (z_i/n_i) + (z_j/n_j) \qquad (4)$$

With n_i as the number of electrons in outermost orbit. Here, b and ρ are the repulsive strength and hardness parameters, respectively. In our calculations value of ionic radii (r_i) and van der Waals coefficients (c_{ij} and d_{ij})have been taken from Singh[9] and co-workers[11-19].The values of ρ_{ij} for the rubidium iodide have been taken from Hafemeister and Flygare[20].The values of b for them have been evaluated from the equilibrium condition

$$dW(r) / dr = 0 \qquad \text{at } r=r_o \qquad (5)$$

Using the values of $f(r)$ obtained from the knowledge of overlap integral and its derivatives from the knowledge of overlap integral (5).

$$f(r_0) = f_0 \exp(-r_0\backslash\rho_{+-}) = €_{+-}S_{+-}^2 \qquad (6)$$

$$\text{With } f_0 = A_{+-} (1-2r_+/r_0) \qquad (7)$$

Values of overlap integral (S_{+-}) and constants (A_{+-}) are directly taken from [14]. Values of parameters (ρ_{ij}, b and f_0) have been given in Table 1 together with the equilibrium nearest neighbor distance r_0, which is the only input data used for the calculation of the parameter b.

Phase transition pt can be calculated by difference of interaction potential energies (U1 – U2) divided to the difference in volumes (V2-V1) in two phases.

3. RESULT AND DISCUSSIONS:

TABLE: 3.1 Values of input for ionic crystal.

CRYSTAL	r_0 10^{-8} cm (a)	r_+ 10^{-8} cm (b)	r_- 10^{-8} cm (b)	C_{11} 10^{11} dyne/ cm^2 (a)	C_{12} 10^{11} dyne/ cm^2 (a)	C_{44} 10^{11} dyne/ cm^2 (a)
BN	2.04	1.37	3.00	3.12	1.00	0.14

Table 3.2 Model Parameters for ionic solids

CRYSTAL	ρ	b (in 10^{-12} erg)	f (r)
BN	0.111	0.10	-0.00006

Table 3.3 Values of Cohesive Energies In Boron nitride and phase transition value (Pt)

CRYSTAL	Experimental Value	Theoretical Value
BN(U1-U2)	**186.11**	180.01
BN (Pt) BN(V2-V1)	**3.3** **4**	3.0 3.2

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions. ᵢ, Bi, Ci, Di (i=1, 2).Those parameters are the same as those defined by Verma and co-workers[4] except for the difference that we have included the effect of short range Vander Waals attraction and represented the overlap repulsion by the HF potential. With the knowledge of parameters and input data we have calculated the phase transition, interaction potential energies of boron nitride using their relevant expressions reported (4, 5).

Results obtained in the table are in good agreement with the experimental results which shows that the agreement between experimental and our theoretical results are better.

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