THE COMPRESSION BEHAVIOUR OF AlN NANOCRYSTAL

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Abstract: The expression for the Equation Of State (EOS) is derived using the *ab initio* pseudopotential approach from the variationally determined valence electron eigen values and charge densities. It is obtained by modifying the Misra-Goyal formulation, widely used in the literature to study the elastic properties of solids. The relation is used to study the compression behavior of Aluminium Nitride (AlN) nanocrystal (10 nm and 45 nm). The results obtained with the help of devolved EOS are compared with the available experimental data.

INTRODUCTION

Aluminium Nitride (AlN) has various unique properties such as excellent thermal conductivity, high chemical resistance, high melting point, wide band gap and small electron affinity, which have gained considerable interests [1-5]. As for bulk AlN, high-pressure studies have proved that a pressure-induced wurtzite to rocksalt phase transition occurs at the pressure of about 20.0 GPa [6,7]. However, perhaps no theoretical work has been done so far to investigate such transition in AlN nanocrystal. Thus, in the present paper we have derived the analytical expression for bulk modulus from the ab-initio pseudopotential (PP) approach to the total nanocrystal energy within the framework of Density Functional (DF) formalism and have used it to analyze the phase transition of AlN nanocrystal of 10 nm and 45 nm size.

THEORY

The expression for the total crystal energy in momentum space is particularly designed to be applicable with the pseudopotential method and a plane-wave basis set. A plane wave basis set is used to represent the (pseudo) valence wave functions. Such a basis set describes the charge density in the valence region to the same degree of accuracy for different crystal structures. In other words, the basis is not biased toward a particular crystal structure, which is usually difficult to achieve in other choices of basis sets. Furthermore, the angular dependence of the charge density is well accounted for, and there is no need for a spherical averaging procedure of the charge density which may introduce appreciable error in describing highly directional covalent bonds. The present formalism, however, is readily applicable to calculations with mixed basis sets (e.g. plane wave plus Gaussian) as well.

Using the *ab initio* pseudopotential approach the expression for the EOS is derived from the variationally determined valence electron eigen values and charge densities. The pseudopotential formalism explicitly projects the large and geometry-insensitive core contributions. The Density Functional formalism for the exchange and correlation potential is self consistently employed in the derivation.

The total crystal energy per atom can be written [8-] in momentum space as:

$$E = \bar{\varepsilon} + \left[\mu_{XC}\left(\bar{G} = \bar{0}\right) + \frac{U_{PS}\left(\bar{G} = \bar{0}\right)}{\Omega_a} \right] Z + \gamma_{Ewald} - \frac{1}{2}\Omega_a \sum_{\bar{G}}{}' V_H\left(\bar{G}\right)\rho\left(\bar{G}\right) + \Omega_a \sum_{\bar{G}}{}' \left[\varepsilon_{XC}\left(\bar{G}\right) - \mu_{XC}\left(\bar{G}\right)\right]\rho\left(\bar{G}\right) \qquad (1)$$

where the various terms have their usual meaning [8-10].

The pressure $P(\eta)$ as a function of the compression $\eta = V/V_o$ can readily be calculated using the following relation:

$$\begin{aligned} P(\eta) &= -E' \\ &= \frac{1}{3V_o}\left[\frac{2B}{\xi^2 V_o^{2/3}}\left(\eta^{-5/3} - \eta^{-1/3}\right) - \frac{A}{\xi V_o^{1/3}}\left(\eta^{-4/3} - \eta^{-1/3}\right) + \frac{3C}{\xi^3 V_o}\left(\eta^{-2} - \eta^{-1/3}\right) \right] \end{aligned} \qquad (2)$$

where $\xi = (3/4\pi)^{1/3}$ and prime denotes differentiation w.r.t. volume (V).

The constants A, B and C are eliminated using the expressions for the equilibrium isothermal bulk modulus K_o and its first and second pressure derivatives K_o' and K_o'' respectively. The Eq. (2), then, gets transformed into:

$$P(\eta) = \frac{K_o}{20}\left[\alpha\left\{6\eta^{-2} - 15\eta^{-5/3} + 10\eta^{-4/3} - \eta^{-1/3}\right\} + \beta\left\{3\eta^{-2} - 5\eta^{-4/3} + 2\eta^{-1/3}\right\} + \gamma\left\{\eta^{-2} - \eta^{-1/3}\right\}\right] \qquad (3)$$

with $\alpha = 6 + 9K_oK_o'' + (3K_o' - 4)(3K_o' - 7)$, $\beta = 2(3K_o' - 7)$ and $\gamma = 12$

RESULTS AND DISCUSSION

The pressure dependence of volume for AlN nanocrystal (10 nm and 45 nm) is computed with the help of equation (3) using the values of K_o, K_o’ and K_o’’. The results are plotted in Fig (1). It is interesting to note from Fig (1) that a pressure induced wurtzite to rocksalt phase transition starts at 21.5 GPa and completes at 26.8 GPa for the nanocrystals and is in good agreement with the experimental value [11]. The high-pressure measurements on AlN nanocrystals with an average crystal size of 10 nm show that the wurtzite to rocksalt phase transition starts at 14.5 GPa [12].

Moreover, it is clearly showing that the transition pressure of AlN nanocrystals (45 nm) is significantly larger than that in AlN nanocrystals (10 nm) and is also little larger than that in bulk AlN because of volumetric contraction. Hexagonal AlN nanocrystals (45 nm) display an apparent volumetric contraction as compared to the AlN nanocrystals (10 nm) which might induce the difference of transition pressure. Apparently more detailed experimental studies are needed to fully understand this high pressure behavior of nanocrystals.

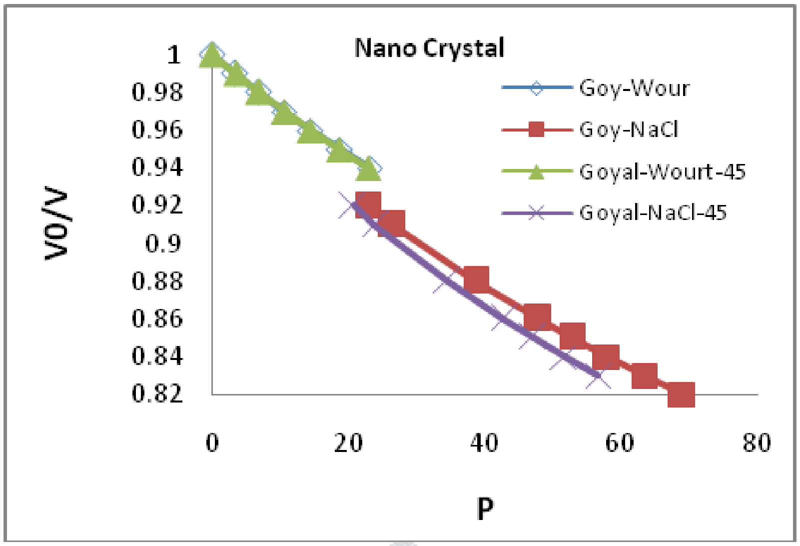

Figure 1: Pressure dependence of the volume of AlN Nanocrystals (10 nm and 45 nm)

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