

Phase Transition and Mechanical Stability of InN Compound

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Ab initio calculations of structural phase transition and mechanical stability of zinc-blende InN compound have been conducted in this work using the pseudopotential plane-wave method within the generalized gradient approximation. The first transition pressure of the material in question has been determined and compared to the data available in the literature. In addition, the mechanical stability criteria have been checked which indicate that zinc-blende InN is mechanically stable for all pressures of interest up to the transition pressure.

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1. Introduction

The group-III-nitrides are of potential interest as optical devices for the optoelectronic technology. This is because of their promising potential to be used for high-temperature, high-frequency, and high-power electronics. These materials are characterized by their wide band gaps and strong bond strength. This makes them being increasingly used for visible light emitting diodes and laser diodes [1–13]. Indium nitride (InN) is an actively investigated semiconductor that has technological applications in optoelectronic devices emitting in the blue light and green ultraviolet spectral regions [14–20]. InN adopts preferentially the hexagonal wurtzite structure, nevertheless, the cubic zinc-blende form has been reported for this material [2, 21–23]. This form has technological advantages, such as easier doping, easier cleaning (for laser facets), and easier contacting.

The study of the effect of high-pressure on the fundamental properties of semiconductors has been increased during the recent years [24–32]. This is mainly due to the development of the diamond anvil cell and a rapid increase in computer power. Although some papers investigated the mechanical properties of InN [14–17, 33], only a few of them dealt with the effect of pressure on these properties. This has prompted us to take up such a study for InN in the zinc-blende structure. Our study is focused on the transition phase and mechanical stability of InN under high-pressure. The calculations are performed using *ab initio* calculations based on the density functional theory (DFT) within the generalized gradient approximation (GGA).

2. Computational method

The calculations are performed using a pseudopotential plane-wave method as implemented in the CASTEP code [34]. The Vanderbilt-type ultra-soft pseudopotentials [35] are used in order to describe the interaction between valence electrons and ion cores of In and N. The GGA of Perdew et al. for solids [36] is used to treat the exchange-correlation energy.

The plane wave cut off energy is taken to be 400 eV. The Brillouin zone integrations are carried out using Monkhorst and Pack k -point meshes [37], with a $12 \times 12 \times 12$ special k points mesh.

The finite strain-stress method [38] is used for determining the single-crystal elastic coefficients (C_{ij}). By deriving C_{ij} , the polycrystalline elastic constants are calculated using the Voigt–Reuss–Hill approximations [39–44].

3. Results and discussion

Thermodynamically speaking, the lowest Gibbs free energy, given by the relation

$$G = U + PV - TS, \quad (1)$$

corresponds to the stability of any given structure. In Eq. (1), U , P , V , T , and S are total internal energy, pressure, volume, temperature, and entropy, respectively. By optimizing the cell parameters and atomic positions for zinc-blende ($B3$) and NaCl ($B1$) phases at $T = 0$ K, one can obtain the pressure-induced structural transition. For that purpose and given the fact that G becomes equal to the enthalpy H at $T = 0$ K, we have studied the variation of H as a function of pressure for both phases being considered here. Our results are displayed in Fig. 1. Note that the two curves representing H versus pressure for $B3$ and $B1$ phases cross at a pressure of 8.35 GPa. This suggests that the InN zinc-blende phase transforms to

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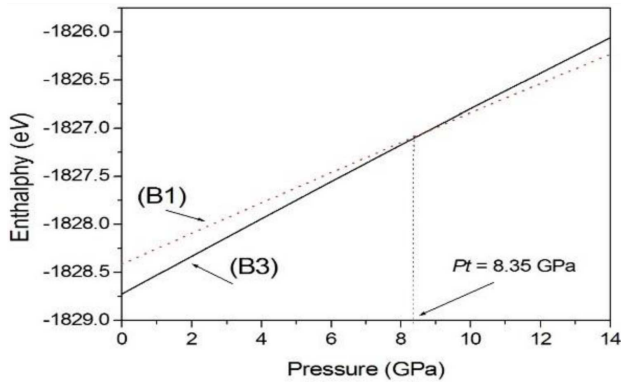


Fig. 1. Enthalpy versus pressure for zinc-blende (B3) and NaCl (B1) phases of InN.

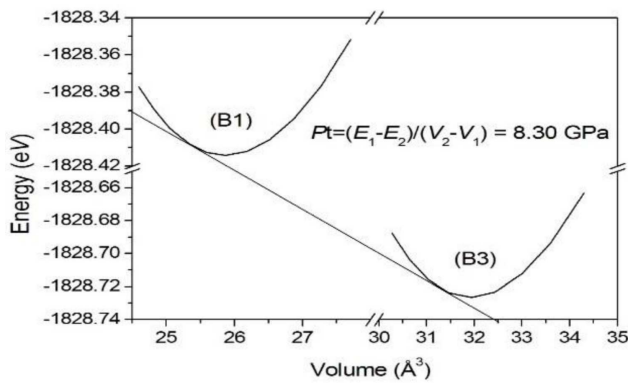


Fig. 2. Total energy versus volume for zinc-blende (B3) and NaCl (B1) phases of InN.

the NaCl phase at a transition pressure P_t of 8.35 GPa. Beyond P_t , the NaCl phase becomes more stable than the zinc-blende phase.

The value of P_t can also be obtained from the curves of total energies and relative volumes in B3 and B1 phases. In this method, P_t is the gradient of common tangent given by [45]:

$$P_t = -\frac{\Delta E}{\Delta V} = \frac{E_1 - E_2}{V_2 - V_1}. \quad (2)$$

In the current contribution, the total energies versus relative volumes for both InN phases of interest are illustrated in Fig. 2. Our findings show that $P_t = 8.30$ GPa. This value is very close to the one we obtained via enthalpy. As compared to transition pressures reported in the literature for zinc-blende InN, our findings seem to be smaller than those lying in the range 12.1–23.0 GPa, as suggested by Adachi [46].

The elastic constants of solid materials are important parameters that are critical for device fabrications and various fundamental properties of the materials are related to them [47–50]. In this work, the elastic constants of zinc-blende InN have been calculated. Our results yielded values of 168, 113, and 83 GPa for C_{11} , C_{12} ,

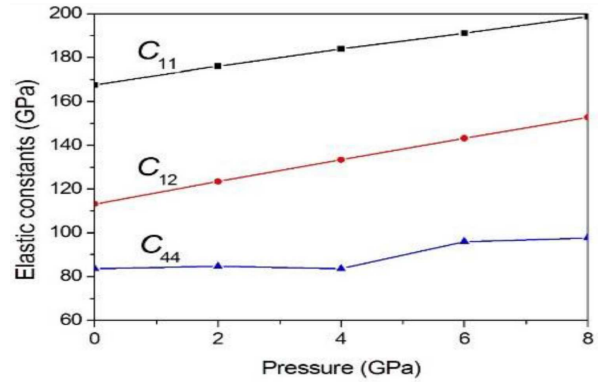


Fig. 3. Elastic constants versus pressure for zinc-blende (B3) InN.

and C_{44} , respectively. These values are respectively in reasonably good accord with those of 187, 125, and 86 GPa reported by Wright [17] using DFT calculations. The pressure dependence of these elastic constants is shown in Fig. 3. Note that all elastic constants of interest increase with enhancing pressure. The behavior appears to be linear for C_{11} and C_{12} , but non-linear for C_{44} .

In order to check the mechanical stability of the material in question under pressure, we have used the traditional mechanical stability criteria for cubic crystals under pressure [31, 43],

$$K = \frac{1}{3}(C_{11} + 2C_{12} + P) > 0,$$

$$G = \frac{1}{2}(C_{11} - C_{12} - 2P) > 0, \quad G' = C_{44} - P > 0. \quad (3)$$

Our findings showed that all the criteria are fulfilled for each given pressure of interest. This indicates that zinc-blende InN is mechanically stable for all pressure up to P_t .

4. Conclusion

In summary, based on *ab initio* pseudopotential plane-wave method within the GGA, the pressure dependence of structural and elastic properties of InN were investigated. Our results showed that InN transforms from B3 to B1 at a pressure of about $P_t = 8$ GPa. The material of interest is found to be mechanically stable up to a pressure of P_t .

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