An interface study of c-BP/c-GaN heterostructure

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We present the modeled a superlattice for cubic-GaN on BP structure at (001) direction. The modeling procedure was achieved by using first principle calculations based on the density functional theory with Plane Wave Self Consistent Field. We also report the total energy of ground state, lattice constant, electronic band structure and potential energy line up of heterojunction between c-BP/c-GaN compounds. The effects of interface have been investigated in this system.

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1. Introduction

Boron monophosphide (BP) and gallium niride (GaN) are III-V compound which are cubic with the zinc blende structure. BP has an indirect band and wide gap semiconductor and BP has an important role for electronic and optical applications [1-3].

GaN is a wide direct band gap semiconductor which has some applications such as light-emitting diodes (LEDs) [4,5], laser diodes, UV detectors and microwave power, ultra-high power switches [6]. Therefore, GaN has a strong impact in the production of these electronic devices.

Lattice constants of cubic BP and cubic GaN are 8.5784 a.u and 8.5236 a.u respectively. Their lattice mismatch is less than 0.6% [7] and both BP and GaN are called lattice matched semiconductors. Thus, c-BP is one of the III-V compounds semiconductors and it is grown on GaN to from a lattice-matched heterojunction [8]. BP can be used to growth of GaN on some substrates such as Si [7] that a high uniformity has between BP and GaN. So, BP is used as a buffer material between GaN and Si.

A lot of properties of atoms, molecules, crystals, surface and their interactions can be calculated by using density functional theory (DFT) which is one of the most widely used methods for "ab initio" [9]. Besides DFT which ground on the charge density as the relevant physical quantity is a ground-state theory and it has a highly successful in describing structural and electronic properties of atoms and molecules. Therefore DFT has become a crucial theory in first-principle calculations aimed at describing or even predicting properties of molecular and condensed matter systems [10]. DFT gives us a good description of ground state properties, practical applications are based on approximations which is called exchange-correlation potential at Generalized Gradient Approximation (GGA).

We have reported a detailed calculation of c-BP/c-GaN and have investigated the hetero-interface between the BP and the GaN by using first principle calculations based on DFT at GGA. We have obtained ground state of heterostructure with influence of strain by using z optimization of c-BP/c-GaN. Finally, we have observed the effect of lattice matched on electronic band structure and potential energy line up for c-BP/c-GaN heterojunction at ground state.

2. Theoretical method

DFT proposed in the 1960's by Hohenberg and Kohn [11] and Kohn and Sham [12] provided a simple method for describing the effects of electron-electron interactions. Hohenberg and Kohn first proved that the total energy of an electron gas is a unique functional of the electronic density. The minimum value of the total energy density functional is the ground-state energy of the system and the density yielding this minimum value is the exact ground-state density.

The calculations are based on pseudo potential–total energy scheme using the GGA in the form of Perdew-Burke Emzerhof (PBE) [13,14]. The exchange-correlation potential describes the effects of the Pauli principle and the Coulomb potential with electrostatic interaction of the electrons.

We used the Plane wave self consistent field code (PWscf) [13] and the electronic potential average technique in our calculations. PWscf, available as a part of quantum-espresso [15] based on DFT, is used for the total energy calculations. The electrostatic potential average is calculated via the electronic density n (r). Firstly, introduce the plane-averaged electronic density $\bar{n}(z)$:

$$\bar{n}(z) = \frac{1}{S}\int_S n(r)dxdy \qquad (1)$$

where z axis is perpendicular to the slab surface S. The macroscopic-average electronic density $\bar{\bar{n}}(z)$:

$$\bar{\bar{n}}(z) = \frac{1}{d}\int_{-d/2}^{d/2} \bar{n}(z+z')dz' \qquad (2)$$

where is defined from the plane-averaged density by integration over the interplanar distance d of the slab. The electrostatic potential V(r) is related to the total charge density, including ionic charge via the Poisson equation. The plane-average potential $\bar{V}(z)$ is related to its and macroscopic average $\bar{\bar{V}}(z)$:

$$\bar{\bar{V}}(z) = \frac{1}{d}\int_{-d/2}^{d/2} \bar{V}(z+z')dz' \qquad (3)$$

as seen ref. [16].

In these calculations, the plane wave basis sets with a kinetic energy cut-off number 40 Ry and k points (12x12x6). These parameters are determined by total energy minimization calculations of system. Electrostatic macroscopic potential average and electronic band structure are calculated to investigate the effect of interface of superlattice.

3. Results and discussion

We have modelled c-BP/c-GaN bulk heterostructures as monolayer in direction of (001). The bulk heterostructure for c-BP/c-GaN system is shown in Fig. 1. The monolayer superlattice structure has been derived from one unit cell cubic zincblende BP compound and one unit cell cubic zincblende GaN compound by modelling in the z direction. The lattice constants of these models have been determined by making z optimization of system. After that we have carried out relaxation effect on atomic positions. In this result of calculation, the total energy and the average effective potential of the system have been achieved for monolayer.

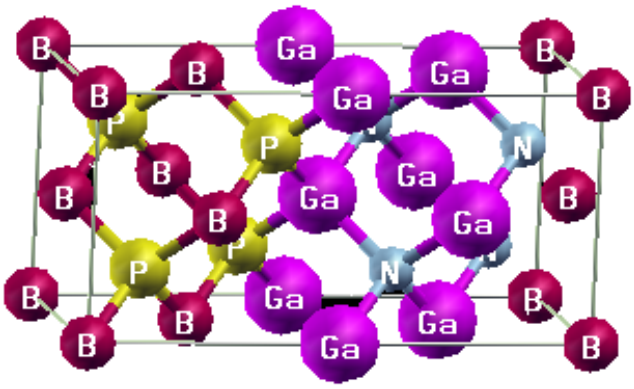

Fig. 1. Bulk heterostructure for c-BP/c-GaN system.

c-BP/c-GaN superlattice which is modelled as monolayer the (001) direction have been investigated by the minimization of total energy. In the Fig. 2, equilibrium lattice constant is calculated as 8.6473 a.u.

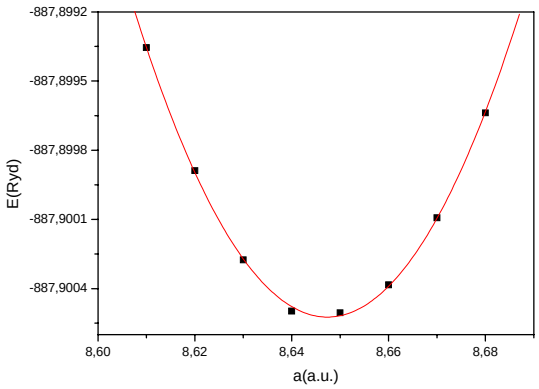

Fig. 2. Total energy as a function of the lattice constant for the monolayer c- BP/c-GaN bulk heterostructure.

In Fig. 3, we present the potential curve and macroscopic average potentials for the bulk system. The macroscopic average potential difference is very small (0.0078 Ryd) that it has calculated at influence of strain for monolayer c-BP/c-GaN bulk heterostructure. In this system, the macroscopic average potential, the bulk character at both sides of the interface and lattice constant matching are significant properties for using BP as a buffer material.

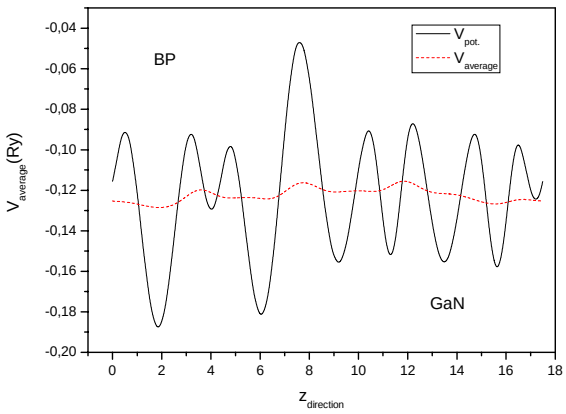

Fig. 3. Macroscopic average potential for c-BP/c-GaN bulk heterostructure.

The electronic band structure has important for bulk heterostructure. In Fig. 4, we have calculated electronic band structure along the special k-points in the Brillouin zone which include in R, Z, Γ, X, M and Γ points for c-BP/c-GaN system. It can be seen that there are two forbidden energy gap in the Fig. 4.

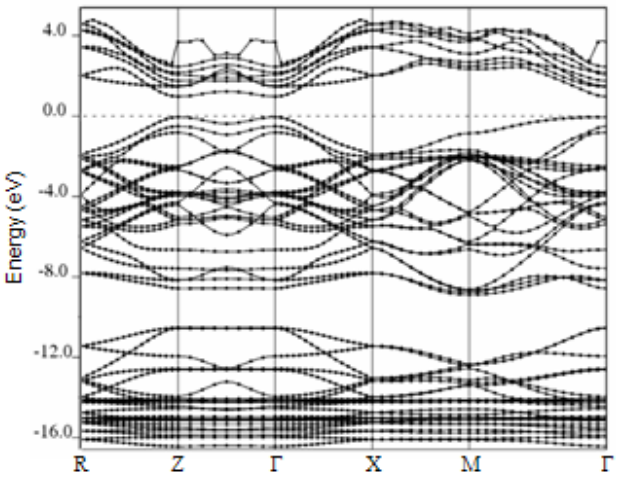

Fig. 4. Electronic band structure for c-BP/c-GaN bulk heterostructure.

4. Conclusions

We present an interface study of lattice-matched c-BP/c-GaN bulk heterostructure using first principle total energy calculations which is based on the DFT. We have determined equilibrium state of system via z optimization of superlattice. Thus, we have carried out the potential energy line up and the electronic band structure for this system.

It is clear that there is a minimum average effective potential difference at interface between BP and GaN compounds. For this reason, BP has an important role a buffer material to product consists of GaN electronic and opto-electronic devices. GaN is very useful for optical communication devices.

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