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Electronic and structural properties of large lattice-mismatched Si/BP superlattice

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We present results for electronic and structural properties of large lattice mismatched Si/BP superlattice by first principle calculations based on the density functional theory. A self-consistent pseudopotential calculation has been performed at Si/BP (001) strained interface. We also analyze the total energy of ground state, lattice constant and electrostatic potential line up of heterojunction between Si/BP zincblende compounds. Finally, we have investigated electronic band structure and the effect to electrostatic potential line up of structural details at interface of this system.

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1. Introduction

Over the past few decades, there has been increasing interest in wideband gap semiconductors. There are III-V and II-VI compound semiconductors with high band gap such as AlN, GaN, BN, BP [1-4] and the only high bandgap materials in group IV are diamond and silicon carbide (SiC) [5].

It is impossible to imagine solid-state physics without semiconductor heterostructures. This heterostructures take an important place in the development of semiconductor technology. Especially heterostructures consisting of silicon are widely used in many fields. Silicon is a desirable material for electronics because of its high crystalline quality, large size and low cost. Silicon has been the mainstay of the electronics for decades. It works as a conducting substrate and also has well characterized electrical and thermal properties. Si(001) is the important material in the complementary metal oxide semiconductor (CMOS) industry [6], so it is preferred for electronic and optoelectronic devices based on gallium nitride.

GaN is used to make blue LEDs [7,8] and lasers [9,10]. Due to its wide bandgap, GaN offers breakthrough solutions in the application field. GaN layers with cubic crystal symmetry can be grown on substrates such as silicon carbide or sapphire [11,12]. But these substrates are costly and can't meet the other requirements. GaN on Si is foundation to the development of low cost and high performing power devices [13-15] and LEDs. Si(001) is favored for GaN growth due to several reasons: it is the material of the Si industry and wanted for a possible integration of GaN devices with Si electronics. It is easier to etch by wet chemical etching, and easier to cleave [16]. But the major problem occurs due to the thermal and lattice mismatch between Si and GaN [17]. This situation causes GaN cracking. Thermal and large lattice mismatches of Si with GaN prevents the growth of high quality GaN films. So, Si has not been a good material for GaN growth. Therefore a suitable layer called buffer layer between Si and GaN is necessary. Buffer layer is important that the strain is be minimized. Boron monophosphide (BP) is one of the most promising materials for such a buffer layer [18] which enables to obtain smooth. BP has about 16% lattice mismatch to Si and the lattice mismatch between GaN and BP is less than 0.6%. As a buffer layer, aim of BP thin layer enables to growth GaN on Si. Associated with growth tecniques for BP on Si, a lot of experimental study has been carried out [19-22] but any theoretical study has been met.

Density functional theory (DFT) is one of the most widely used methods for "first-principles" calculations of the structure of atoms, molecules, crystals, surfaces and their interactions [23]. DFT has become a common tool in first principles calculations aimed at describing or even predicting properties of molecular and condensed matter system [24]. Also the method has proved to be highly successful in describing structural and electronic properties in a vast class of materials ranging from atoms and molecules to simple crystals to complex extended systems.

In this paper, a theoretical interface study between Si and BP are investigated by using first-principles numerical simulations. We have also discussed bulk heterostructure and electronic properties of zincblende Si/BP. The aim of this work is to observe the effects of large lattice-mismatch between monolayer Si and monolayer BP on the atomic structure and electrostatic potential line up. Finally we have calculated electronic band structure Si/BP (001) in the tetragonal Brilouin zone (BZ) of super lattice.

2. Method of calculations

First-principles calculations were performed by using the Plane Wave Self Consistent code (PWSCF) [25]. Generalized gradient approximation (GGA) in the form of

Perdew-Burke-Ernzerhof (PBE) was used for exchange–correlation potential in the total energy calculations [26,27]. All structures have been treated within supercell geometry using the periodic boundary conditions. A plane wave basis set with kinetic-energy cutoff of 40 Ryd. has been used. In the self-consistent potential and total-energy calculations, the Brillouin zone is sampled by special **k** points. The numbers of these **k** points are (6×6×6) for bulk Si, BP and (12×12×6) for Si/BP heterostructures according to the size of superlattices. All atomic positions and lattice constants are optimized by using the conjugate gradient method, where the total energy and atomic forces are be minimized. The pseudopotentials having three, five and four valence electrons for Boron (B: $2s^2 2p^1$), Phosphorus (P: $3s^2 3p^3$) and Silicon ions (Si: $3s^2 3p^2$) were used respectively.

In the modelling of Si/BP heterostructure, we have used one unit cell Si and one unit cell BP compound and the macroscopic average technique in the average electrostatic potantial calculations for Si/BP superlattice [28].

3. Result and discussion

We consider the crystal structures of Si and BP have zincblende lattice form. The unit cells of these lattice forms are shown in the Fig. 1.

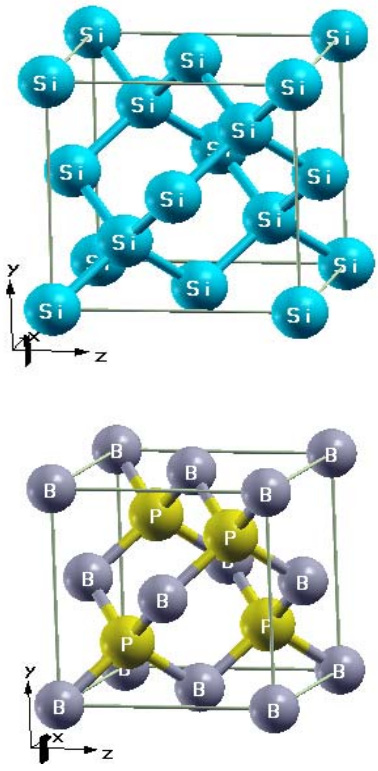


Fig. 1. Crystal structures of Si and BP.

For Si and BP, lattice parameters are determined by total energy with respect to cubic lattice constant a. Total energy as a function of lattice constants is presented in the Fig. 2. We found $a_{Si} = 10.34\ a.u$ and $a_{BP} = 8.60\ a.u$ by using the total energy as a function of the lattice constant in the Fig. 2.

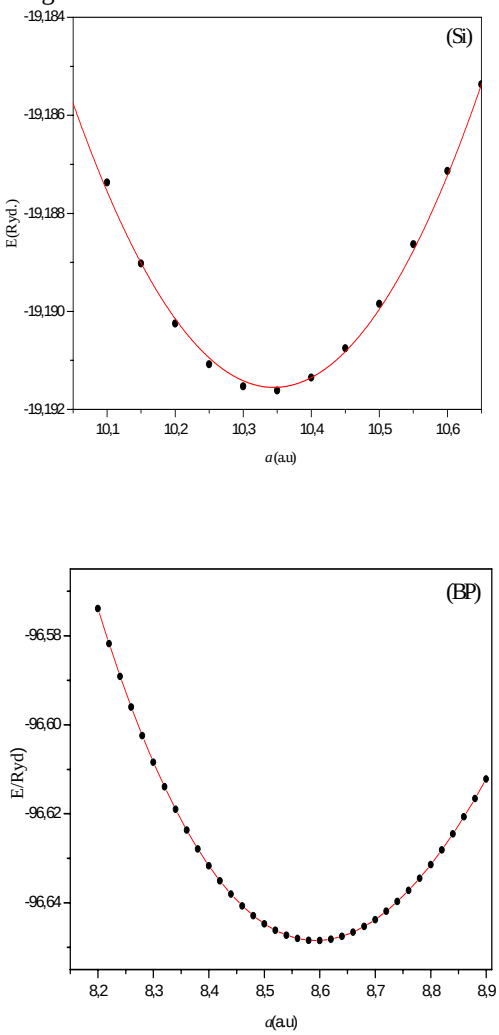


Fig. 2. Total energy as a function of the lattice constant for Si and BP.

Si/BP superlattice which is modelled as monolayer in the (001) direction have been investigated. The lattice constant of modelled this system has been determined by the minimization of total energy. Equilibrium lattice constant is calculated as $a_{Si/BP} = 9.49\ a.u$ from Fig. 3. According to this value, Si atoms are compressive strain and BP atoms are tensile strain. The extension of the Si/BP superlattice system has been calculated by extending in the z direction and compressing in the x,y direction and also compressing in the z direction and extending x, y direction.

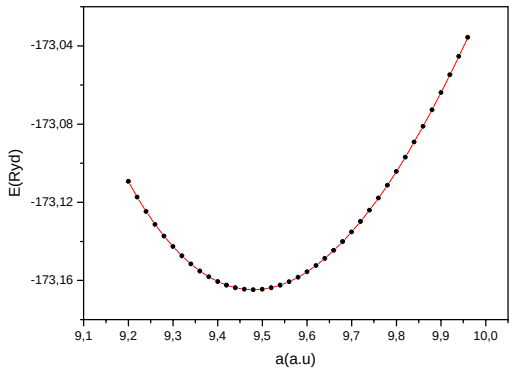


Fig. 3. Total energy as a function of the lattice constant for Si/BP.

In the result of optimization, while the atomic positions are decreasing in proportion to $0.0992\,a_{Si/BP}$ for x and y directions, they increase in proportion to $1.0122\,a_{Si/BP}$ for z direction. These optimization values have been affected to all atomic positions. Before relaxation, this superlattice heterostructure has been shown in the Fig. 4(a). After relax total energy calculation, atomic positions of the system has been shown in the Fig. 4(b).

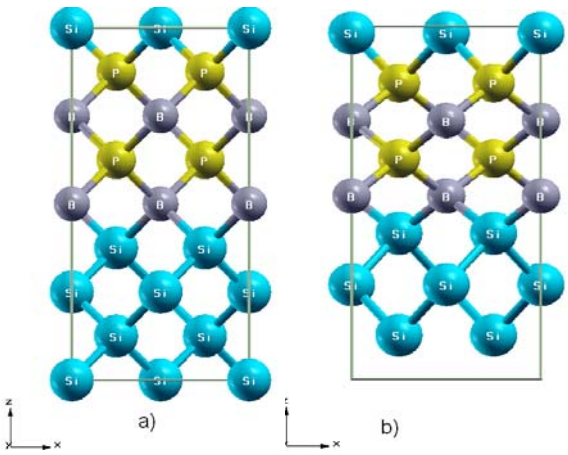
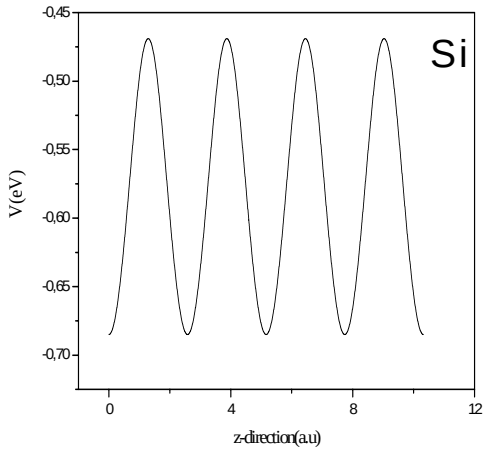


Fig. 4. Bulk heterostructure for Si/BP system: (a) Before relaxation, (b) After relaxation.

It is clear that after relaxation, interatomic distances significantly have changed in terms of before relaxation in the Fig. 4. Also it is obvious that the change of atomic positions result from strain effect of large lattice mistmatched between Si and BP. The average electrostatic potentials are presented for Si and BP in the Fig. 5.



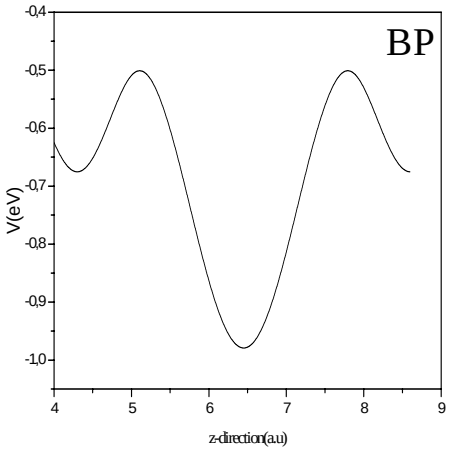


Fig. 5. Electrostatic potentials for zincblend Si and BP.

The result of calculation shows that the average electronic potentials are obtained from a supercell calculation. Also, both electrostatic potential curves of Si and BP are periodic, have regular forms. The supercell size is enough to reproduce the bulk-like character at both sides of the interface and the effect of the relaxation of the atomic positions at the interface region due to the strain related with the lattice constant mismatch of the Si/BP.

We have carried out calculations for large lattice mismatched Si/BP superlattice in the (001) direction to investigate the role of the interface. In the Fig. 6, we present the average electrostatic potential $\overline{V}(z)$ along the super lattice axis of Si/BP.

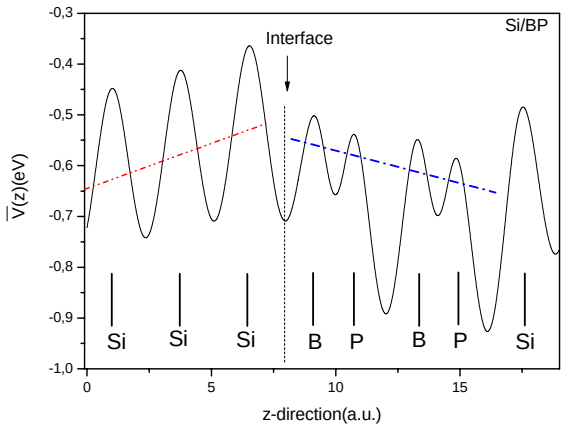


Fig. 6. Average electrostatic potential for zincblend Si/BP monolayer superlattice heterostructure.

Due to interface effects, the mean value of $\overline{V}(z)$ shows a sawtooth form with a clear tilt. While the mean value of $\overline{V}(z)$ is increasing in the the left side, it decreases on the right side of the interface region. In the left of interface region, the biggest value mean of $\overline{V}(z)$ is -0.54 eV and its lowest value is -0.65 eV. On the other hand, in right of interface region, the biggest value mean of $\overline{V}(z)$ is -0.57 eV and its lowest value is -0.72 eV.

Finally, the electronic band structure is shown for Si/BP monolayer superlattice heterostructure along high symmetry points in the Fig. 7. It can be seen that the energy bands are very dense between -2eV and 2eV. In the region, valance and conduction bands are too close each other and the band gap is very small. This situation shows that the Si/BP heterostructure has good electrical conductivity.

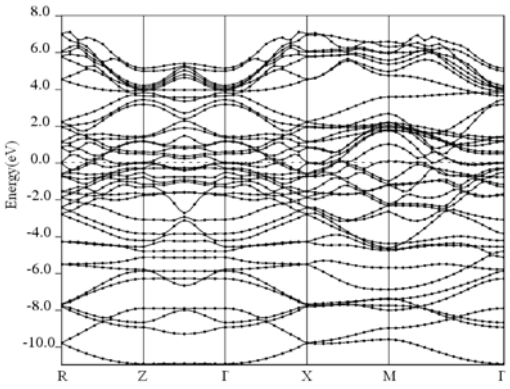


Fig. 7. Electronic band structure of Si/BP monolayer superlattice heterostructure.

4. Conclusions

We present a theoretical study of the structural and electronic properties of large lattice-mismatched Si/BP bulk heterostructure using first principle total energy, average electrostatic potential and electronic band structural calculations based on the density functional theory. We determined a sawtooth form with a clear tilt for the mean value of $\overline{V}(z)$ at interface between Si and BP compounds. It is clear that BP is one of the most important materials as a buffer layer for GaN on Si. These materials are qualified in the production of electronic and optoelectronic devices.

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