EFFECT OF Ge-DOPING POSITION ON THE ELECTRONIC BAND STRUCTURE OF InP NANOWIRE

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Abstract

In this study, the effect of Ge-doping on the electronic band structure of [111] oriented zinc-blende InP nanowires has been investigated using first-principles calculations based on density functional theory. The pure and H-passivated nanowires are formed to have a diameter of 1.5 nm. The doped InP nanowires are modeled by changing the position of the Ge atom. In place of In and P atoms, which are removed separately from different positions of the nanowire, Ge atoms are substituted. In order to determine the electronic properties, the band structures of all nanowires have been calculated. It is shown that the band structures obtained in the doping made by removing the In atom exhibit the character of an n-type semiconductor, while the band structures obtained in the doping made by removing the P atom form a p-type semiconductor.

Keywords: InP nanowire, Ge doping, first principles calculations.

INTRODUCTION

Semiconductor nanowires composed of III-V group elements attracted considerable attention due to their electronic and optical properties [1-4]. These nanostructures are building blocks in technological applications such as field effect transistors, light-emitting diodes, and biological sensors [5-7]. InP has excellent potential for application to these devices because of its direct band gap characteristic, high electron mobility, and absorption efficiency [8-10].

Nanowires are called one-dimensional structures that differ from their bulk counterparts due to the large surface-volume ratio and quantum confinement effects. Also, the charge carriers are confined in two directions. Because many applications of nanowires are based on the transport of the carriers, the control of transport properties is very significant in these structures. The transport properties of nanowires can be altered by introducing foreign impurities, and new electronic, mechanical, optic, and magnetic properties are obtained from nanowires.

Many experimental and theoretical studies have been performed to determine the electronic and structural properties of InP nanowires. The methods of metal–organic vapor epitaxy, laser ablation, and chemical beam epitaxy are used to synthesize InP nanowires [11-13]. Theoretically, the dependence of the band gap on the nanowire's diameter changing was investigated [14]. To eliminate the surface effects, the passivation of the surface with hydrogen atoms was carried out [15,16]. The doping effect on InP nanowires was studied to understand the electronic, magnetic, and optic properties [17-19].

In this study, the electronic band structures of InP nanowires are studied by doping Ge and varying the dopant positions using first principles method.

METHOD

The first principles calculations have been implemented using Quantum Espresso software package based on density functional theory [20-22]. Exchange and

correlation potentials are included using the generalized gradient approximation (GGA) of Perdew, Burke and Enzerhof (PBE) [23]. The plane wave cut off energy is taken as 40 Ry for InP nanowires, and the number of k points in Brillouin zone is set as 1x1x6 Monkhorst-Pack points. All geometries have been optimized until the forces are less than 0.025 eV $A^{\circ -1}$.

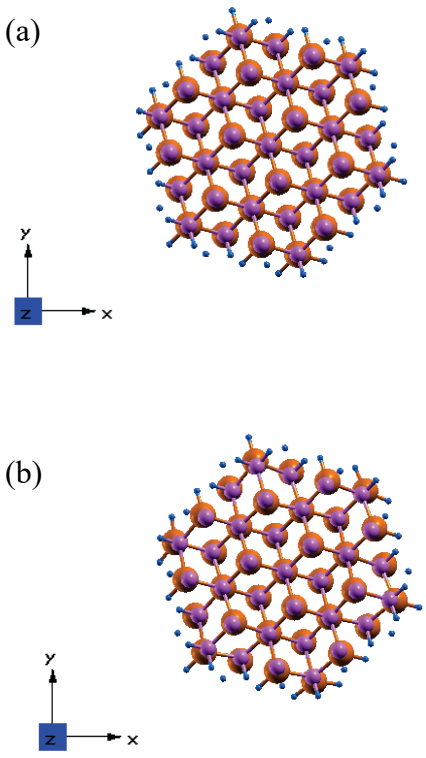

Fig. 1. *The top views of InP nanowires (a) before (b) after optimization (The orange, purple and blue balls are In, P and H atoms, respectively)*

The optimization calculations have been performed for bulk InP in the zinc-blende phase. InP nanowire with 1.5 nm diameter has been formed along [111] direction using optimized bulk parameters. The dangling bonds of the surface atoms are passivated by hydrogen atoms in order to eliminate the surface effect. Periodic boundary conditions are applied along the z-axis, and sufficient vacuum space (15 Å) is taken to avoid interaction between InP nanowires. The top views of pure InP nanowires before and after optimization are shown in Figure 1.

Ge doping has been made by removing atoms from different positions of the InP nanowire, which has been passivated with hydrogen atoms. The top and side views of Ge-doped InP nanowires are shown in Figure 2.

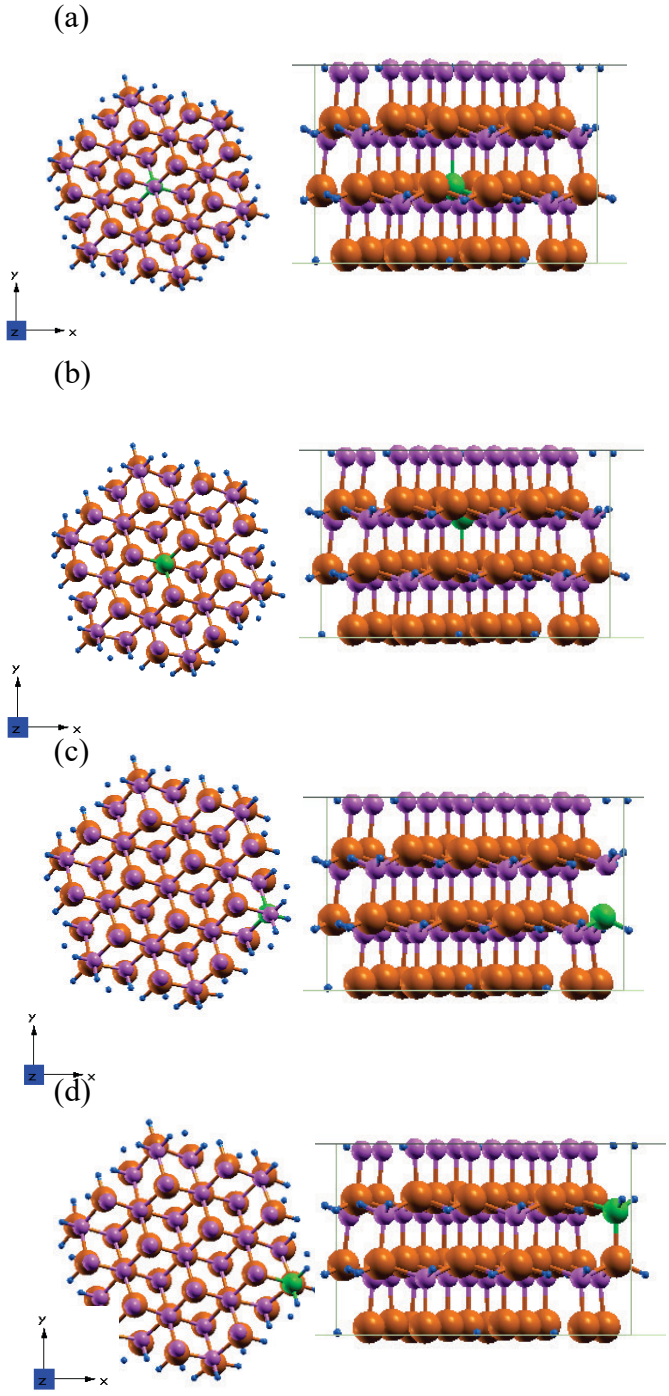

Fig. 2. *Top and side views of doped InP nanowires with Ge atoms at different positions (Orange, purple, green and blue balls are In, P, Ge and H atoms, respectively)*

RESULT AND DISCUSSION

Before the calculation, the structural and electronic properties of bulk InP have been tested first. The lattice constant and electronic band structure have been calculated. The lattice constant is obtained as 6.01 Å consistent with the previous studies [24]. The band gap of bulk InP is direct and found as 0.43 eV in accordance with theoretical studies [25]. InP nanowire is modelled by using the parameters of bulk InP.

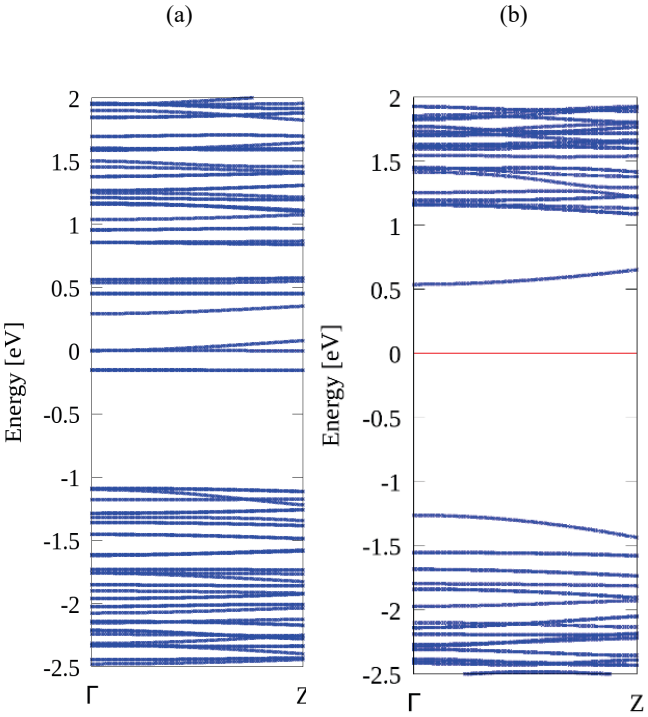

Fig. 3. *Band structures for pure (a) unpassivated (b) H-passivated InP nanowires*

Figure 3 shows the electronic band structures of pure unpassivated and H-passivated InP nanowires. In order to eliminate the dangling bonds which introduce energy levels around the Fermi level, the surface atoms of the nanowire are passivated with hydrogen atoms. Thus, the localized bands created by dangling bonds are disappeared. As can be seen from the figure, when the surface atoms are passivated with hydrogen, the band gap opens up, and it is calculated as 1.80 eV.

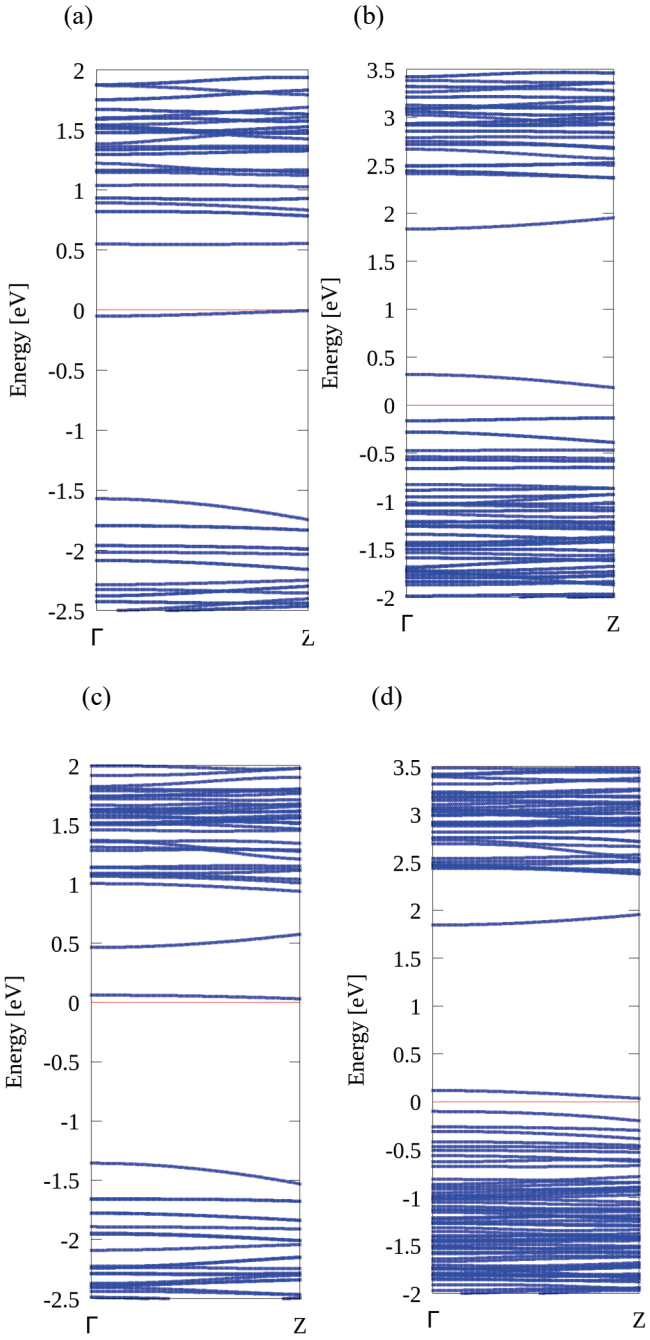

Fig. 4. *Band structures of Ge doped InP nanowires with Ge atoms at different positions.*

The electronic band structures of Ge-doped InP nanowires are shown in Figure 4. In order to investigate the electronic properties, Ge is added to replace the In and P atoms extracted separately from different positions of the InP nanowire. Firstly, the Ge atom is substituted for the In atom in the nanowire's centre, and the nanowire's electronic band structure is calculated and shown in Figure

4a. The horizontal red line sets the fermi level as zero point. The figure shows that Ge doping creates a donor level below the conduction band. The Fermi level is located around the conduction band. The energy band gap is found as 1.61 eV. It can be seen the band gap narrows compared to the pure InP nanowire. In the second stage, the P atom in the centre of the nanowire is removed, the Ge atom is substituted, and the band structure is determined. Figure 4b shows that the electronic band gap narrowed slightly compared to the electronic band gap of the nanowire in Figure 4a and is found as 1.52 eV. The Fermi level falls into the valence band. Also, valence band maximum and conduction band minimum energy values shift to higher energy levels in this nanowire. Figure 4c shows the electronic band structure of the InP nanowire formed by substituting a Ge atom instead of the In atom on the nanowire surface. When Figure 4c is examined, it is seen that the donor level, which occurs similarly to Figure 4a, maintains its existence. The electronic band gap is found as 1.39 eV, and it has an indirect bandgap unlike that of other nanowires. The Fermi level is located next to the conduction band. The electronic band structure of the nanowire obtained as a result of Ge doping instead of the P atom on the surface of the InP nanowire is given in Figure 4d. Compared to Figure 4b, it can be said that there is little widening in the electronic band gap, and it is measured as 1.73 eV. Similarly, the Fermi level enters the valence band levels. While the conduction band minimum energy value remained at the same level, the valence band maximum energy level decreased slightly.

CONCLUSION

The effect of Ge doping position on the electronic band structure of InP nanowire has been investigated by using first principles calculations. The energy band structures have been calculated, and results show that all InP nanowires have semiconductor characteristics. According to the observed electronic properties depending on the position of the dopant atom, there is no significant change in the electronic band gap. Valence band maximum and conduction band minimum energy have higher values in Ge-doped InP nanowires substituted with P atoms than in Ge-doped InP nanowires substituted with In atoms. Also, It is shown that the band structures obtained in the doping made by removing the In atom exhibit the character of an n-type semiconductor, while the band structures obtained in the doping made by removing the P atom form a p-type semiconductor.

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