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Investigation on the Electronic Structures of in Doped GaN by First-principles Calculation

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Abstract

GaN is regarded as the pioneer leading the semiconductor technology revolution and the core technology supporting the development of new energy, electronic information, national defense and military industry and other strategic emerging industries. However, the low p-type effective doping concentration of GaN materials greatly limits the improvement of the performance of GaN based devices. In this paper, the crystal constant, energy band structure and density of states of In doped GaN are revealed by first principle calculations, and are compared with the undoped GaN. The results indicated that P-type doping is formed by doping GaN with In by replacing Ga atoms with In atoms. the GaN crystal structure is slightly deformed, the lattice constant is increased, and the band gap width is reduced, the energy level of In p-orbital electrons is lower than that of Ga p-orbital and d-orbital electrons and becomes acceptor level, resulting in a P-type doping.

Keywords

GaN; Dope; First-principles Calculation; Electronic Structure.

1. Introduction

The third generation of semiconductors represented by SiC and GaN, have excellent performances such as high frequency, high efficiency, high power, high pressure resistance, high temperature resistance and strong radiation resistance[1,2]. GaN is a wide energy gap material, which can provide similar performance advantages as silicon carbide (SiC), but the possibility of cost reduction is greater. The industry believes that in the next few years, the cost of GaN power devices is expected to be reduced to the same price as silicon MOSFET, IGBT and rectifier. Due to the growing demand for high-speed, high-temperature and high-power semiconductor devices, the semiconductor industry reconsiders the design and materials used in semiconductors. With the continuous emergence of a variety of faster and smaller computing devices, it is difficult for silicon materials to maintain Moore's law. Because of the unique advantages of GaN materials[3,4], such as excellent noise figure, high maximum current, high breakdown voltage and high oscillation frequency, it provides a unique choice for a variety of applications, such as military, aerospace and national defense, automotive fields, as well as high-power fields such as industry, solar energy, power generation and wind power. Due to the use of gallium nitride optoelectronic semiconductors in military, aerospace, national defense and consumer electronics, optoelectronic semiconductors have become the main product type in the global gallium nitride semiconductor device market and occupy an absolute dominant position.

For a long time, the p-type effective doping concentration of GaN materials is not high, and it is impossible to realize p-type heavy doping[5]. It greatly limits the improvement of the performance of GaN based devices, making carrier injection ratio lower, p-type ohmic contact preparation difficult, luminous efficiency lower, forward operating voltage higher, high-power

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devices generate heat, reliability lower, and so on. Herein we use the first principle calculation to explore the lattice constant, band structure, density of states of In doped GaN.

2. Computational Approach

The first principle calculations were executed by employing the Quantum Expresso (QE). The exchange-correlation terms were indicated with the GGA represented by PBE functional (GGA-PBE). A plane-wave basis set was used to perform the geometry condition and the band structure, the cut-off energy was set as 50 Ray. Every atom was relaxed in the primary cell by the time of the force among the atoms was under 0.001Ray/Å. The convergence criterion for energy was set as 10-8 Ray. A 13×13×7 MP grid was employed for sampling the Brillouin zone for structure relaxation.

3. Results and Discussion

3.1. Crystal Structure and Electronic Structure of GaN

The crystal structure of GaN is shown in Figure. 1. GaN materials crystallize in a tetragonal unit cell. The calculated lattice parameters of GaN are summarized as $a = 6.202\text{Å}$, $c = 10.486\text{Å}$, $c/a = 1.629; \alpha = 90^0, \beta = 90^0, \gamma = 120^0$. It is displayed that the calculated lattice constants are slightly larger than the reported experimental lattice constants.

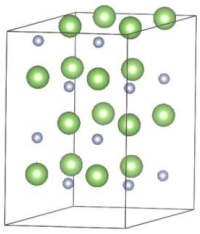

Figure 1. The crystal structures of GaN

The electronic structures of GaN are explored with PBE functionals. A representative band structure of GaN is shown in Figure. 2, the band structures of GaN show same features near the fermi energy. The results show that GaN exhibits a direct band gap, and both valence band minimum (VBM) and conduction band maximum (CBM) locate at Γ point. The VBM at point Γ is two-degree degenerate, which results in a heavy hole and a light hole in the VBM.

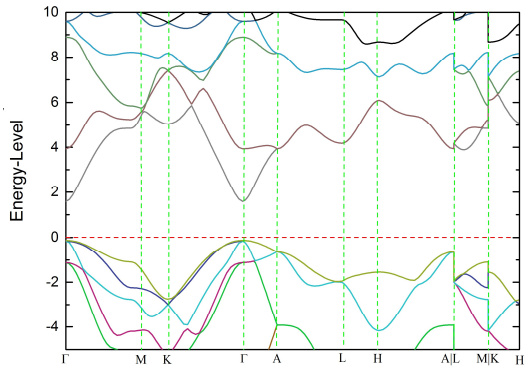

Figure 2. The electronic structures of GaN calculated with PBE + U approach.The Fermi energy is set to 0 eV.

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In principle, the density of state (DOS) diagram can be used as a visualization result of the energy band structure. Figure 3(a) shows the DOS diagram of doped GaN, Figure 3(b) shows the DOS diagram of Ga in undoped GaN, and Figure 3(c) shows the DOS diagram of N in undoped GaN. According to the above 4.3~4.5 three DOS diagrams, the electronic contributions made by Ga atoms and N atoms in undoped GaN crystals in the conduction band of undoped GaN crystals are similar, and the electronic contributions made by N atoms in undoped GaN crystals in the valence band of undoped GaN crystals are greater than those made by Ga atoms, The N atom in the valence band is the main electron that constitutes DOS. From the DOS diagram analysis of undoped Gan, it can be seen that the conduction band is close to the Fermi level, and the s orbit and P orbit of GA atom provide the main electrons, and there are a small number of D orbit electrons. Looking at the valence band close to the Fermi level region, it can be concluded that the main electrons in the valence band of undoped Gan are mainly provided by N atoms, and a small number of electrons are provided by Ga atoms. It can be seen from the DOS diagram that the p orbital electrons in N atoms make the main contribution and the p orbital and d orbital electrons in a small number of Ga atoms provide electrons. It can be seen from the energy band diagram and DOS diagram of undoped GaN crystal that there is a wide band gap, which conforms to the characteristics of semiconductor with wide band gap. The GaN bandgap width will be reduced by doping to improve the application of GaN materials.

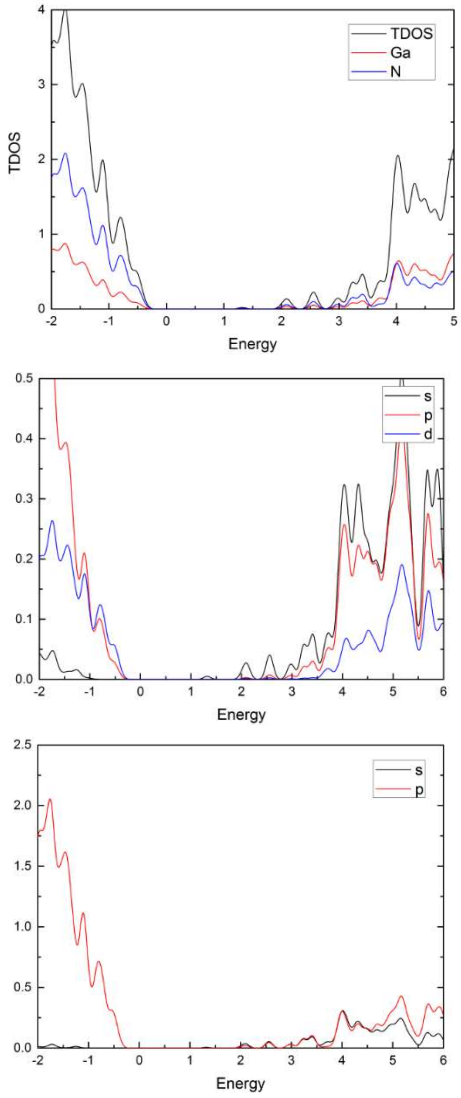

Figure 3. Temperature dependence of electrical conductivity of LaZnPnO (Pn = P, As and Sb)

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3.2. Crystal Structure and Electronic Structure of In-doped GaN

Indium is the same group IIIA transition metal element as Ga, which is widely used in the doping modification of semiconductor materials. In this paper, we use In atom to replace Ga atoms in GaN, and the doping has an effect on the lattice constant of GaN. The performance of In-doped GaN materials will be improved by observing the structural schematic diagram, energy band diagram and DOS diagram. After In doping GaN, the valence electrons involved in the simulation are Ga:4s24p1, N:2s22p3, In:5s25p1. The optimized unit cell structure after In doping GaN is shown in Figure 4. For the supercell of In-doped GaN, the structure is also optimized first. The crystal structure of GaN containing In atoms is visualized to obtain the structure diagram, and the properties of solid bonding are analyzed. Lattice constants of In doped GaN crystals calculated by first principle calculation, the result is $a = 6.483\text{Å}$, $c = 10.56\text{Å}$, $c/a = 1.629$; $\alpha = 90^0$, $\beta = 90^0$, $\gamma = 120^0$.

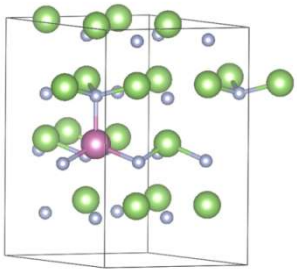

Figure 4. The crystal structures of In-doped GaN

The comparative analysis of the crystal constants of In doped GaN and undoped GaN shows that the value of the crystal constants increases, and the reason for the increase of the crystal constants is that the radius of In atoms is larger than that of Ga atoms. When In atoms combine with N atoms to form In-N bonds, the bond length is longer than that of Ga atoms combine with N atoms to form Ga-N bonds, which causes lattice deformation and increases the lattice constants.

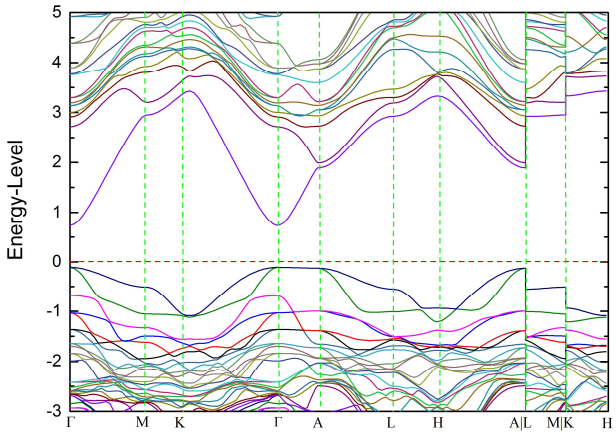

Figure 5. The electronic structures of In-doped GaN calculated with PBE + U approach.The Fermi energy is set to 0 eV.

Figure 5 In doped GaN energy band diagram. From the comparison between Figure 2, it can be concluded that the bottom of the conduction band and the top of the valence band move upward, and the Fermi energy level enters the valence band region. After the substitutional Ga atom is

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doped, the band gap width of the In atom is 0.251eV less than that of the undoped GaN atom, and its band gap width is reduced, which improves the electron transition. In atoms displace Ga atoms in GaN, and a small amount of In impurities are doped into GaN semiconductor materials. The conductivity of GaN semiconductor materials will be greatly improved. Since the semiconductor material without doped GaN is doped with an In with three electrons in the outermost electron, when the In atom forms a covalent bond with the N atom, a hole is added due to the lack of one electron. Each doped In atom has a hole, which is called p-type semiconductor. In p-type semiconductors, holes account for a large number, free electrons account for a small number, holes are most carriers, and the conductivity is enhanced.

From the DOS diagram analysis of In doped GaN in Figure 6, it can be concluded that each atom in In doped GaN mainly provides electrons. In the conduction band region close to Fermi level, Ga atoms and N atoms are mainly provided with electrons and a small number of In atoms, while in the valence band region close to Fermi level, Ga atoms and N atoms are mainly provided with electrons; From the DOS diagram of Ga in In doped GaN in Figure 6, it can be seen that the conduction band of Ga atom in GaN close to the Fermi level provides electrons mainly from the p-orbital electrons of Ga, and the valence band of Ga atom close to the Fermi level provides electrons mainly from the d-orbital electrons of Ga; From the DOS diagram of In in the In doped GaN in Figure 6, it can be seen that the conduction band of the In atom in the GaN close to the Fermi level provides electrons mainly from the p-orbital electrons of In, and the electrons of the p-orbital and d-orbital introduced by the In doped GaN into the new In atom perturb the p-orbital and d-orbital electrons of the Ga atom, making these energy levels transition to the lower energy level and the energy end move, causing the top of the valence band to move down, the energy band to become dense, and the band gap width to narrow. It can be seen that the effect of In doping on the electronic structure of GaN is relatively small.

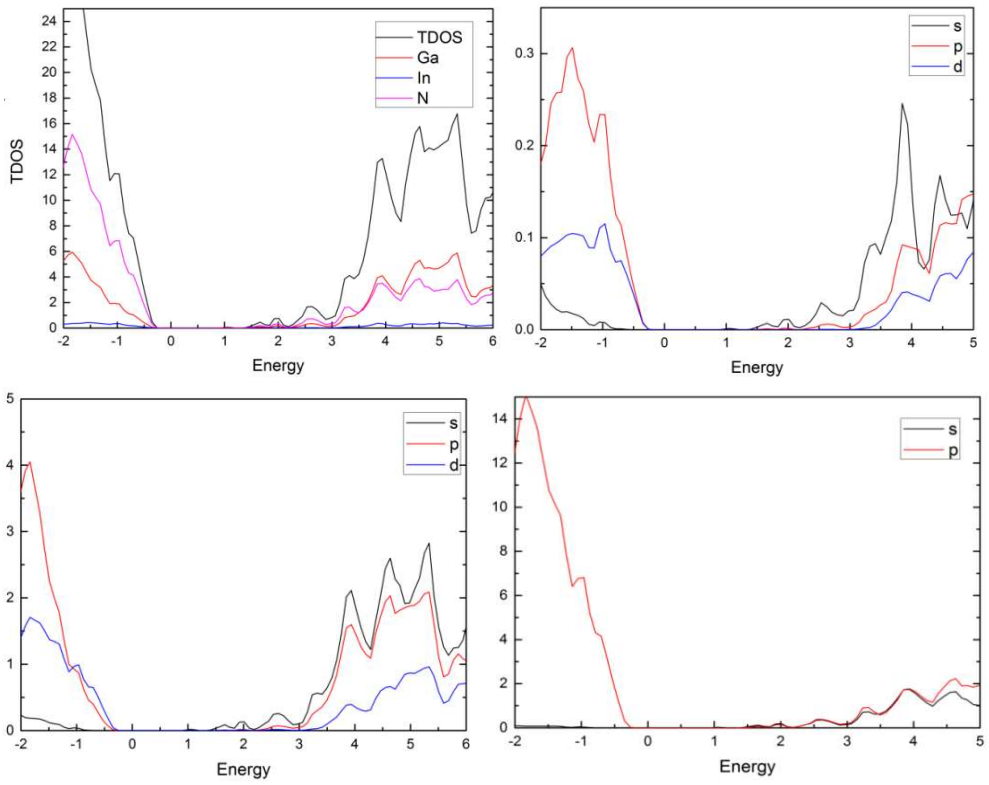

Figure 6. Temperature dependence of the figure of merit ZT for LaZnPnO (Pn = P, As and Sb)

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4. Conclusion

In this paper, undoped GaN and In doped GaN are studied from three aspects: crystal constant, energy band structure and density of states, and the doped GaN is compared with the undoped GaN, P-type doping is formed by doping GaN with In. Doping is carried out by replacing Ga atoms with In atoms. Since the radius of the new atoms doped is larger than that of the original ones, the GaN crystal structure is slightly deformed, the lattice constant is increased, and the band gap width is reduced, so as to achieve the desired doping control purpose. As GaN is widely used in LED lighting, electronic power, radio frequency microwave, mobile phone fast charging, new energy vehicles, rail transit, smart grid, consumer electronics and 5G mobile communication market, GaN is regarded as the pioneer leading the semiconductor technology revolution and the core technology supporting the development of new energy, rail transit, electronic information, national defense and military industry and other strategic emerging industries.

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