Physica E: Low-dimensional Systems and Nanostructures 98 (2018) 191–196

Contents lists available at ScienceDirect

Physica E: Low-dimensional Systems and Nanostructures

journal homepage: www.elsevier.com/locate/physe

Discrete impurity band from surface danging bonds in nitrogen and phosphorus doped SiC nanowires

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ARTICLE INFO

Keywords:
Silicon carbon nanowires
Nitrogen and phosphorus doped
Surface danging bonds
Hydrogen passivation
Electronic and optical properties

ABSTRACT

The electronic structure and optical properties of the nitrogen and phosphorus doped silicon carbide nanowires (SiCNWs) are investigated using first-principle calculations based on density functional theory. The results show doping can change the type of the band gap and improve the conductivity. However, the doped SiCNWs form a discrete impurity levels at the Fermi energy, and the dispersion degree decreases with the diameter increasing. In order to reveal the root of this phenomenon, we hydrogenated the doped SiCNWs, found that the surface dangling bonds were saturated, and the discrete impurity levels are degeneracy, which indicates that the discrete impurity band of the doped SiCNWs is derived from the dangling bonds. The surface passivation can degenerate the impurity levels. Therefore, both doping and surface passivation can better improve the photoelectric properties of the SiCNWs. The result can provide additional candidates in producing nano-optoelectronic devices.

1. Introduction

Silicon carbide (SiC) has obtained increasing attention due to their potential properties for nanotechnology applications [1–8]. Similar to other nanostructures, SiC nanowires (SiCNWs) have been attracted some researchers because it can be applied for Light-emitting diodes (LEDs) [9], lasers [10–12], UV detectors [13], and microwave powers [14], so we can fully utilize their superior performance by handling SiCNWs. For instance, Al dopants in 3C-SiCNWs could favor a more localized state near the Fermi energy, which improves the electron field emissions [15], and Al dopants could cause red-shifts of the photoluminescence band [16]. Via self-propagating high-temperature synthesis [17] and catalyst-assisted pyrolysis of polysilazane precursors [18] prepared N-doped SiC nanoparticles and P-doped SiC nanowire, respectively. Zheng et al. combined the theoretical calculations with the experimental results, which showed the magnetic state is depending on the distance between Fe dopant atoms [19]. In 2015, Zhao et al. put forward that the N content of nanowires could affect the FE properties [20]. The p-type doping in SiCNWs was investigated, they found that the ionization energy of acceptor state is much larger in nanowires than that in the bulk SiC as a result of quantum confinement effect, and Co doping is more suitable method for achieving low-resistivity semiconductors either in nano materials or bulk material [21]. After, the electronic band structure for a [111]-oriented nanowire with total H, OH passivation [22] and a combination of both were studied, the calculations indicated the band gap feature could be changed and reduced [23,24] by surface modification [25]. In 2016 years, B–doped SiCNWs were exhibited a far more improved microwave absorption ability in the frequency range of 2–18 GHz compared with SiCNWs [26]. In 2017 year, Oliveira et al. investigated the mechanical and electronic properties of hydrogen-passivated 3C-, 2H-, 4H-, and 6H-SiCNWs, analyzing the effects of the diameter on these properties [27]. However, there are expected to be very few studies on the simultaneous passivation and doping [28] of 2H-SiCNWs.

To date, most of the studies are focused on the band gap, structural stability, magnetism, and so on [29,30]. However, the impurity levels are produced because of doping, so it is one of a necessary mean for changing some properties. Whereas how to reduce the effect of the impurity levels is seldom studied.

In this paper, we utilize the first principle to research the band gap and the electronic structure of nitrogen (N) and phosphorus (P) doped SiCNWs. Impurity levels occur after doping and the degree of dispersion decreases with the increase of the diameter. In order to study the reason of the dispersion degree decrease, we hydrogenated the doped SiCNWs. This work can change the properties of SiCNWs for applying for some special devices and circuits, in addition of the SiC low-dimensional

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https://doi.org/10.1016/j.physe.2018.01.006
Received 21 December 2017; Received in revised form 9 January 2018; Accepted 10 January 2018
Available online 11 January 2018

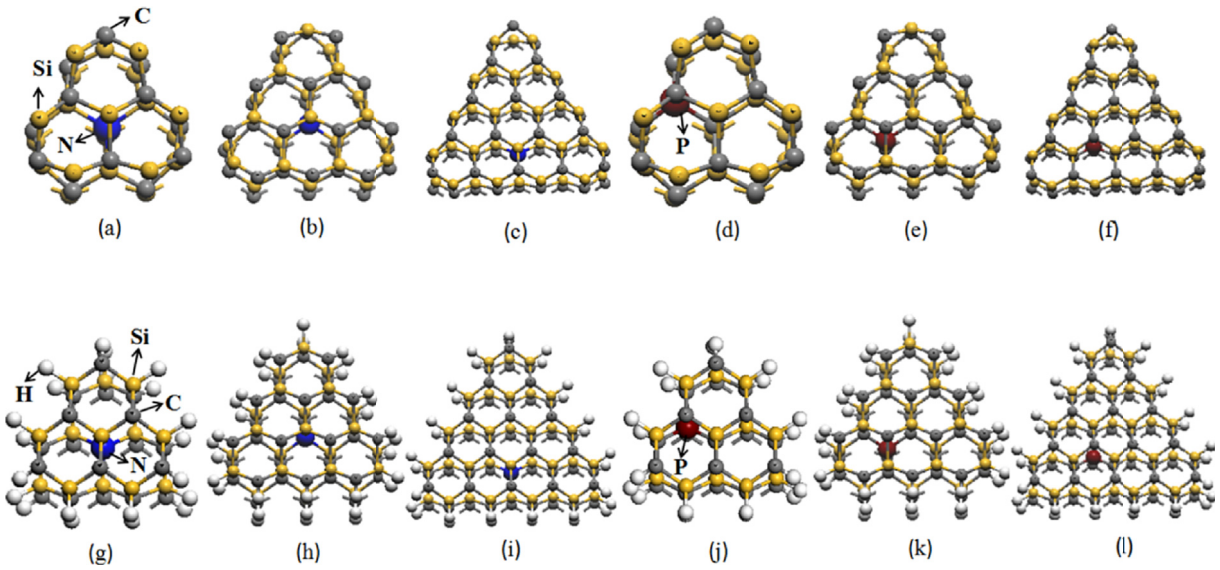

Fig. 1. The SiCNWs are marked as (a) N1-SiCNWs, (b) N2-SiCNWs, (c) N3-SiCNWs, (d) P1-SiCNW, (e) P2-SiCNWs, (f) P3-SiCNWs, (g) Hyd. N1-SiCNWs, (h) Hyd. N2-SiCNWs,(i) Hyd. N3-SiCNWs, (j) Hyd. P1-SiCNWs, (k) Hyd. P2-SiCNWs and (l) Hyd P3-SiCNWs.

materials are very promising for the applications as laser induced nonlinear optical materials [11,12].

2. Computational methods and models

2.1. Computational methods

By using DFT in the CASTEP code of the first principle calculation to optimize the structures, the optimization parameters are as follows:(1) the convergence standard of the individual-atom energy is 2.0×10^{-5}eV, (2) the convergence standard of interaction between electrons is 0.05 eV/Å, (3) the convergence standard for maximum shift of atom is 0.002 Å, and (4) the convergence standard of crystal internal stress is 0.1 GPa. The plane-wave cutoff energy of 600 eV, and the k points was set to $1 \times 1 \times 8$ under the Monkhorst-Pack grid.

2.2. Structural model

The wurtzite structure 2H-SiC as the basic unit ($1 \times 1 \times 1$) is used to establish the structure of nitrogen-doped SiCNWs (N-SiCNWs), phosphorus-doped SiCNWs (P-SiCNWs), nitrogen-doped the passivation SiCNWs (Hyd. N-SiCNWs) and phosphorus-doped the passivation SiCNWs (Hyd. P-SiCNWs). The SiCNWs is along with [001] direction and the nanowires with triangular sections in different diameters as follows see (Fig. 1).

3. Results and discussion

3.1. Structural stability

Cohesive energy can measured the stability of the material structure, and the structure is more stable, the cohesive energy is smaller. The cohesive energies of N- and P-SiCNWs with different diameters can be calculated by Eq. (1)

$$E_B = E_T - E_{Si}N_{Si} - E_C N_C - E_d N_d \quad (1)$$

For Hyd. N- and P-SiCNWs with different diameters, their cohesive energy can be obtained by Eq. (2)

$$E_B = E_T - E_{Si}N_{Si} - E_C N_C - E_d N_d - E_H N_H \quad (2)$$

where E_T is the total energy of the nanostructure, and N represents the number of Si, C, H and doped atom in the structure, E_{Si}, E_C, E_H and E_d express the free energies of Si, C, H and doped atom ($E_{Si} = -101.52$eV, $E_C = -145.84$eV, $E_H = -15.85$eV, $E_N = -261.71$eV, $E_P = -174.33$eV), respectively.

According to the first principle and Eqs. (1) and (2), we obtain several structure parameters of N-SiCNWs, P-SiCNWs, Hyd.N-SiCNWs and Hyd.P-SiCNWs, shown in Tables 1 and 2, respectively.

Seen from Tables 1 and 2, The c decreases with the increase of the diameter after passivation, therefore, which is contrary before passivation. The radius of P is larger than that of N, so the cohesive energy of P-SiCNWs and Hyd. P-SiCNWs are larger than that of N-SiCNWs and Hyd. N-SiCNWs, respectively. The cohesive energy of N-SiCNWs and P-SiCNWs is smaller than that before doping. Likewise, the Hyd. N-NWs and Hyd. P-NWs is smaller than N-SiCNWs and P-SiCNWs. For doping, the structure is more stable after passivation, which indicates that for the stability of the structure, the role of the dangling bond is greater than doping on SiCNWs.

The diameter of nitrogen atom is larger than the carbon atom (the diameter of the phosphorus atom is larger than that of silicon atom), so

Table 1
The lattice structure parameters of N-SiCNWs and P-SiCNWs with various diameters.

SiCNWs structures	Lattice constant c (Å)	Bond distance L (Å)	Diameter D (Å)	Total energy E_T (eV)	Cohesive energy E_B (eV)	Impurity concentration N_d(10^{20}/cm^3)	Danging band concentration N_D (10^{22}/cm^3)
N1	5.081	1.862	6.254	−3514.16	−182.61	15.20	2.70
N2	5.089	1.960	9.171	−5872.54	−314.75	6.669	1.60
N3	5.09	1.892	12.270	−8758.10	−479.35	4.886	1.46
P1	5.072	1.859	6.246	−3468.54	−180.05	15.31	2.75
P2	5.086	1.818	9.175	−5826.93	−312.20	6.662	1.60
P3	5.090	1.858	12.254	−8712.57	−476.88	4.896	1.47