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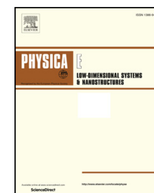

# Effect of surface dangling bonds on transport properties of phosphorous doped SiC nanowires

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ABSTRACT

Based on the semiconductor transport theory, a computational model for the axial conductivity of one-dimensional nanowires is established. Utilizing the band structure data from the first principles, the conductivity, carrier concentration and mobility of phosphorus doped SiCNWs (P-SiCNWs) before and after passivation were numerically simulated. The results show that hydrogen passivation can greatly improve the conductivity of P-SiCNWs, above room temperature, the conductivity is improved nearly two orders of magnitude, and enhance the thermal stability. The reason is that hydrogen passivation saturates the surface dangling bonds, leading to the disappearance of discrete impurity band of P-SiCNWs. In addition, the surface dangling bonds lead to greater thermal instability of conductivity under room temperature, but this thermal instability decrease rapidly with the increase of temperature. The study will help us to understand the transport properties of low dimensional semiconductors, and provide theoretical support for the research of nano electronic and optoelectronic devices.

## 1. Introduction

Silicon carbide (SiC) nanomaterials, it has the advantages of high band gap width, high critical breakdown electric field, thermal conductivity, small dielectric constant, high electron saturation mobility, strong antiradiation ability and other good mechanical properties [1–4], which is widely used in high frequency, high power, high temperature, radiation resistant electronic and optoelectronic devices [5–8]. For example, the SiC nanowires exhibit room temperature photoluminescence, making it an ideal material for making blue LED and laser diodes [8–11]. SiC nanomaterials have excellent characteristics such as low threshold field strength, high current density, high temperature stability and so on, which is expected to be used as an electric field emission material. Utilizing this characteristic, it can be used to create the third generation of new electronic light source [12], and will play a great role in image display technology. In addition, SiCNWs has wide application prospects in hydrogen storage [13], biomedicine [14], sensor [15], microwave absorption and electromagnetic shielding [16,17]. As we all know, the semiconductor conductivity is closely related to the transport process of carriers. Therefore, studying the transport properties of the semiconductor nanomaterials and solving the key problems of nanoelectronic devices have a great significance of the development for the next generation of electronic technology. Up to now, the photoelectric properties of SiC nanomaterials have been extensively studied, but the transport properties and migration mechanism of SiC nanomaterials have rarely been reported [18–21].

In recent years, we have studied with different morphologies and different sizes of SiCNWs and doped SiCNWs [22–25], which found that the surface dangling bonds have an obvious influence on the band structure and electronic density of states [24]. Especially for phosphorus doped SiCNWs (P-SiCNWs), the presence of the surface dangling bonds will lead to the discretization of the impurity band [25], which indicates that P-SiCNWs before and after passivation will have different transport properties and migration mechanism. In this article, based on the previous research results, we simulated the transport properties and migration mechanism of P-SiCNWs and hydrogen passivated P-SiCNWs (Hyd.P-SiCNWs) with different diameters, and the role of the surface dangling bond on the transport process of P-SiCNWs is revealed.

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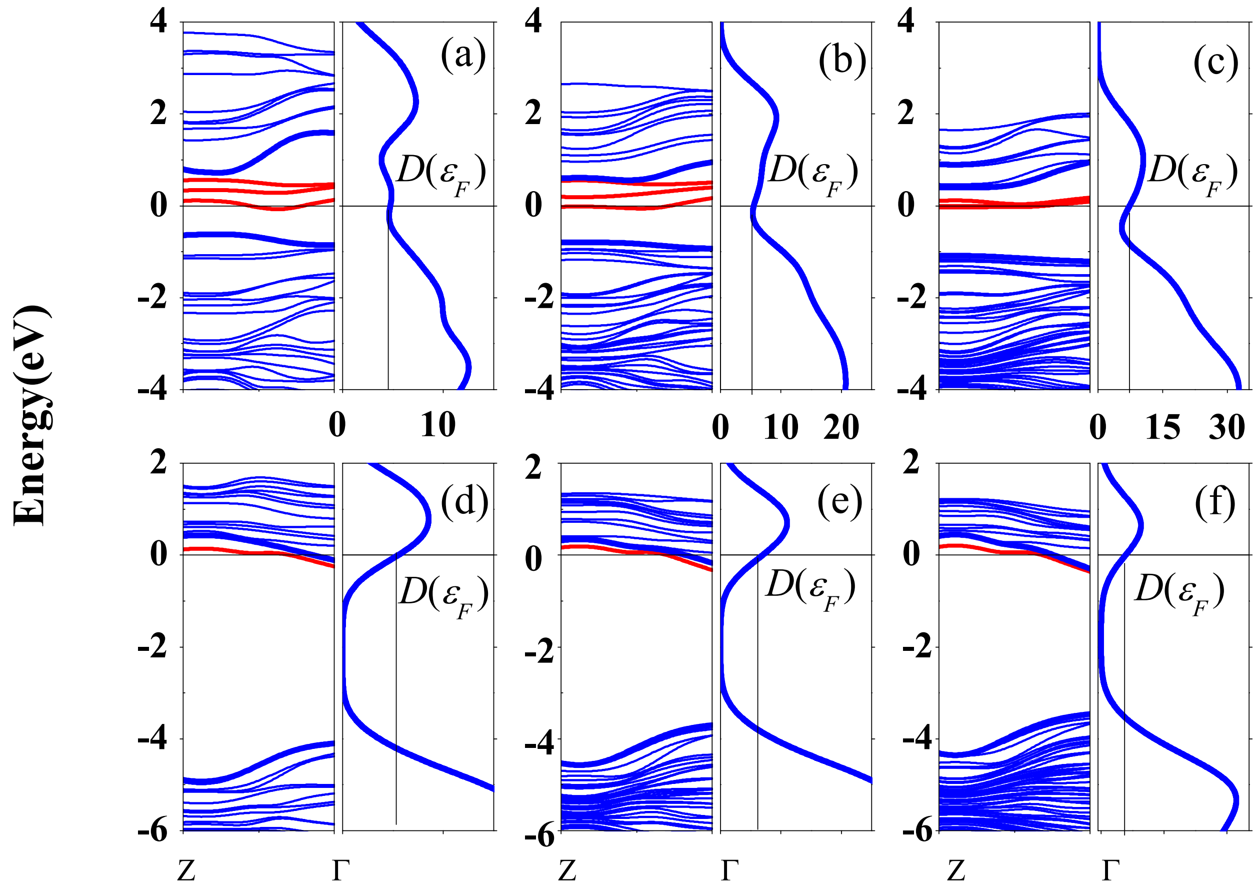


**Fig. 1.** Band structure and density of electronic states. (a), (b) and (c) are P-SiCNWs, and (d), (e) and (f) are Hyd.P-SiCNWs, respectively.

## 2. Transport theory of P-SiCNWs

### 2.1. Band structure and density of electronic states

In the previous work [22,24,25], we constructed supercell, made nanowires along the direction of [001] growth and removed excess atoms, hydrogen atoms were used to passivation surface dangling bonds, and phosphorus atoms were used to replace silicon atoms for structural optimization. By studying the photoelectric properties of P-SiCNWs with different diameters, we obtain the band structure and density of electronic states of P-SiCNWs (P1, P2 and P3, respectively) and Hyd. P-SiCNWs (Hyd.P1, Hyd.P2 and Hyd.P3, respectively), as shown in Fig. 1. In order to highlight the electron state $D(\varepsilon_F)$ at the Fermi level, the scale value of the state density axis is small, making the originally very small $D$ value seems to be very large. Therefore, the band gap shown by the density of electronic states is slightly smaller than that of the energy band.

As can be seen from Fig. 1, the Fermi level passes through the conduction band of Hyd. P- SiCNWs, and exhibits degenerate n-type semiconductor characteristics. As the diameter increases, the conduction band of Hyd. P-SiCNWs moves down, the ionization energy ($\Delta E = E_F–E_C$) increases, but the increase is modest (0.25 eV–0.36 eV). The impurity levels of P-SiCNWs are discretized because of the dangling bonds on the surface, which is manifested as the broadening of the impurity band under the conduction band. At the same time, the Fermi level passes through the impurity band, and with the increase of diameter, the ionization energy decreases considerably (0.1025eV–0.0379eV). Obviously, the migration mechanism of P-SiCNWs changed due to the surface dangling bonds.

### 2.2. Conductivity of phosphorus doped SiCNWs

#### 2.2.1. Axial conductivity of a nanowire

The carriers of the nanowire drift along the axial direction under the axial electric field $\boldsymbol{E}$. Assuming the carrier distribution function is $f(x, p; t)$, the increment of the number of carriers with $t$ to $t + \mathrm{d}t$ and $\mathrm{d}x\mathrm{d}p$ is given as follows

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial p}\frac{\partial p}{\partial t} = \frac{\partial f}{\partial t} + v\frac{\partial f}{\partial T}\nabla T - eE\frac{\partial f}{\partial p}. \tag{1}$$

The electron distribution does not change with time in steady state, that is $\frac{\partial f}{\partial t} = 0$. The temperature gradient is zero in thermal equilibrium state for the nanowire. According to the relaxation time approximation, the distribution function of the number of electrons can be written as

$$f = f_0 + e\tau vE\frac{\partial f_0}{\partial \varepsilon}, \tag{2}$$

where $f_0$ is the electron equilibrium distribution function (Fermi distribution function), $\tau$ and $\varepsilon$ represent relaxation time and electron energy, respectively. In the energy range $\varepsilon \sim \varepsilon + \mathrm{d}\varepsilon$, electronic states of the nanowire can be written as follows

$$D(\varepsilon)\mathrm{d}\varepsilon = \frac{2L}{h}\left(\frac{m^*}{2}\right)^{1/2}\varepsilon^{-1/2}\mathrm{d}\varepsilon, \tag{3}$$

The current density along the axis of the nanowire is

$$j = \left[\frac{2e^2}{Sh}\left(\frac{m^*}{2}\right)^{1/2}\int_0^\infty \tau v^2\varepsilon^{-1/2}\frac{\partial f_0}{\partial \varepsilon}d\varepsilon\right]E. \tag{4}$$

Based on Ohm's law, the axial conductivity of a nanowire can be written as follows

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