Theoretical study of the electronic band gap in $\beta$-SiC nanowires

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The structure and electronic properties of $\beta$-SiC nanowires in the directions of growth [111] and [001] are carried out by means of density functional theory (DFT) based on the generalized gradient approximation (GGA). The dangling bonds of the surface atoms in the quantum wires are passivated using hydrogen atoms. The calculations show that both nanowires exhibit a direct energy band gap at center of Brillouin zone. The electronic band structure and band gaps show a significant dependence on the diameter, orientation and surface passivation.

Keywords: Density functional theory; nanowires; silicon carbide.

La estructura y las propiedades electrónicas de nanoalambres de $\beta$-SiC crecidos en las direcciones [111] y [001] son calculadas a través de la teoría del funcional de la densidad (DFT) basada en la aproximación de gradiente generalizado (GGA). Los enlaces rotos de los átomos de la superficie en los alambres cuánticos son pasivados usando átomos de hidrógeno. Los resultados muestran que ambos tipos de nanoalambres presentan una brecha de energía directa en el centro de la zona de Brillouin. La estructura de bandas electrónica y la brecha de energía muestran una significativa dependencia del diámetro, orientación y pasivación de la superficie.

Descriptores: Teoría del funcional de la densidad; nanoalambres; carburo de silicio.

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1. Introduction

The study of low-dimensional quantum structures has attracted great attention recently in the field of semiconductors research [1–3]. Nanowires are one of the most common one-dimensional (1-D) structures and many kinds of materials can be synthesized into nanowires structures. They present remarkable different properties and applications from their corresponding bulk forms [4]. An example, of these 1-D systems are SiC nanowires (NWs), due to their wide band gap with high electron mobility, SiCNWs would be favorable for applications in high temperature, high power, and high frequency nanoscale devices [5, 6]. In recent years SiC have been intensively studied for their potential applications in electronic devices and sensors [7]. In this work, we study the hydrogen-passivated $\beta$-SiC NWs oriented along both [001] and [111] directions [Figs. 1(a) and 1(b), respectively] using the density functional theory (DFT) based on the pseudopotential plane-wave approach with the supercell technique. The generalized gradient approximation (GGA) exchange-correlation functional used is a revised version of Perdew, Burke, and Enzerhof (RPBE) [8]. We are focusing on the electronic structure and energy gap and their dependence on wire diameter and orientation. Also, the total and partial density of states (DOS) as well as the total electron density are calculated.

2. Calculation procedure

As we have mentioned above, our calculations were performed in the framework of DFT-GGA utilizing the RPBE exchange and correlation functional. The core electrons are described using ultrasoft Vanderbilt pseudopotentials [9] within the CASTEP code [10, 11], as implemented in the Materials Studio software suite. The kinetic energy cutoff for the plane-wave basis set is 280 eV. The Brillouin zone has been sampled with a highly converged set of $k$ points, using grids up to $(1 \times 1 \times 6)$ points according to the Monkhorst Pack scheme [12], the initial bond lengths of Si-H and C-H are 0.147 nm and 0.107 nm, respectively. Nanowires are then placed in a cubic simulation cell with periodic boundary conditions. The size of the simulation cell is chosen so that

![Figure 1](image-url)
THEORETICAL STUDY OF THE ELECTRONIC BAND GAP IN $\beta$-SiC NANOWIRES

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nanowire direction for SiCNWs with similar width $d$. Notice that in both cases the SiCNWs have a direct band gap. This is true for all NWs widths considered here. It is worth noting that dangling bond-like states do not appear within the energy band gap region for SiCNWs in the two directions. This is an indication of hydrogen passivation of the surface dangling bonds that provides a smooth termination of the orbitals.

Figure 3 shows the calculated total density of states (DOS) and partial density of states (PDOS) corresponding to electronic band structure of Fig. 2. An analysis of the orbital contributions shows that the eigenvalue near the valence-band maximum are pure carbon atom $p$ states. Notice that in all cases, (a)-(c), the conduction band edge near the Brillouin zone center is primarily formed by $p$ states, the contribution of $s$ states being negligible.

As expected from quantum size effects, we observed that the absolute value of the conduction band minimum increases in energy as the thickness of the wire decreases. This effect of quantum confinement of electron is observed all widths we studied. This leads to an increase in the electronic energy band gap ($E_g$) with decreasing NWs diameter.

For NWs with similar diameter but different orientation we observed, in Fig. 4, that $E_g$ is greater for wires along [001] and lower for wires along [111] directions. Besides this dependence of $E_g$ on the diameter $d$ and the orientation of growth axis, other ways for modifying the electronic properties would be important for applications. The orientation anisotropy in $E_g$ reduces with the nanowire width and is expected to disappear for very thick wires when the $E_g$ approaches that of the bulk material.

Figures 5 and 6 show the isosurface (a) and the contour map (b) for the total electron density of the two kinds of nanowires [001] and [111], respectively. The electron densities cover regions in the [001] nanowire only for carbon atoms in transversal planes (observed from the [110] perspective) of growth direction. The substantial difference with [111] nanowire is the orientation of these planes, which is diagonal (observed from the same perspective) to the growth direction. In the contour maps, the lighter regions
are associated with higher field values. In the isosurfaces, the darker values correspond to more populated regions. This information could be corroborated observing the contour maps for both wires. As was expected the greater magnitude values are associated with the nearest regions of the more electronegative nucleus (carbon atoms). Consistently, partial density of states [Fig. 3 (a)-(c)], for the superior edge of valence band has a primordial \( p \) character contribution, which are related with carbon atoms shown in the electron density maps. Similarly, the partial density of states for the lower edge of conduction band has a \( p \) character, we suppose that these are related with unoccupied \( p \) orbitals of Si atoms.

4. Conclusions

In summary we have studied, in the framework of density functional theory within the generalized gradient approximation, the structures of \( \beta \)-SiC nanowires oriented in the [001] and [111] and their electronic band structure as a function of diameter. These properties are strongly influenced by quantum confinement. Direct fundamental band gaps are found at Gamma point for both wires, which enlarge as diameter shrinks. It is also found that [001] wires have overall a larger gap than [111] wires. SiC nanowires with direct band gap are promising candidates for optoelectronics applications such as light emitting devices and photodetectors. The wave length of the emitted or detected light can be tuned through the choice of the NWs width.

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