

Structural properties of SiC zinc-blende and wurtzite nanostructures: Atomistic tight-binding theory



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ABSTRACT

The electronic structures of SiC nanostructures consisting of nanocrystals and nanorods are theoretically investigated by atomistic tight-binding model including sp^3s^* orbitals, spin–orbit coupling and the first-nearest neighboring interaction. The excitonic energies and states are numerically computed by the configuration interaction (CI) description of the coulomb and exchange effect. Based on this atomistic model, single-particle gaps, excitonic gaps, coulomb energies and exchange energies of SiC nanocrystals and nanorods are analyzed as a function of diameters and aspect ratios, respectively. The comparison of the results obtained from different structures (zinc-blende and wurtzite) is theoretically reported with the aim to address the importance of the geometric structures on these detailed computations. The simulation emphasizes that the calculations of the electronic structures are mainly sensitive with the shapes, dimensions and geometric structures. The numerical results summarize that the efficient manipulation of structural properties for SiC nanostructures is theoretically accomplished by changing shapes, sizes and geometric structures. Ultimately, the atomistic information of shapes, sizes and structures in the structural properties of SiC nanostructures will be considerably implemented to SiC-based applications.

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1. Introduction

The detailed investigations of the nanostructures have currently fascinated the great attraction in the field of semiconductor research. Nanocrystals and nanorods are considered as the most common zero-dimensional nanostructures which can afford several applications. Silicon carbide (SiC) is one of the most important wide band gap semiconductors because of its excellent thermal conductivity, high breakdown field strength, excellent physical and chemical stability [1–4] and stable and efficient light emission [5]. Bulk SiC presents the poor optical properties because of its indirect band gap. However, when SiC forms the cluster with several or tens nanometers, the improvement of the optical properties is significantly obtained. It has been found that SiC nanostructures are the promising systems for the novel applications in optoelectronic devices [5] and biological labels [6]. Recently there are numerous reports demonstrating the synthesis of SiC nanostructures, while there are a few theoretical studies determining the electronic structures of SiC nanostructures. For example, Deokar et al. [7] presented 3C–SiC nanocrystals synthesized by thermal annealing of SiO_2/Si wafers in CO_2 gas. The obtainable

SiC nanocrystal sizes were in the range 10–60 nm. Selvan et al. [8] successfully prepared porous silicon carbide with fiber like morphology by a hard templating approach using the mesoporous silica SBA-15 as template and sucrose as carbon precursor. SiC nanostructures were high crystalline and displayed porous structures with excellent textural characteristics. Li et al. [9] synthesized the cubic SiC nanowires with diameters of 10–30 nm and lengths up to tens of micrometers by chemical methods. A large blue-shift was observed in the visible photoluminescence. The colloidal cubic SiC nanocrystals with an average dimension of 4.4 nm were fabricated by Li et al. [10] with anisotropic wet chemical etching of micro-sized cubic SiC powder. Their results could afford the building blocks of nanostructure devices as violet light sources and new biological probes in life science. Javan [11] studied a typical spherical SiC nanocrystal ($\text{Si}_{43}\text{C}_{44}\text{H}_7$) with a diameter of 1.2 nm by pseudopotential density functional calculation. The author found that the electronic and optical properties of the $\text{Si}_{43}\text{C}_{44}\text{H}_7$ nanocrystal were impacted by fluorine and oxygen impurities. In addition, Shi et al. [12] presented theoretical absorption spectra of 3C–SiC nanocrystals with different sizes and different surface termination foreign atoms using the semi-empirical PM3 localized-density-matrix method. The calculated results demonstrated that the absorption spectra were clearly sensitive with sizes. Peng et al. [13] presented the band-gap variation

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and stability energy in SiC nanoclusters with different polytypes and dimensions using density functional theory (DFT). These theoretical studies demonstrated that the structural and electronic properties were sensitive with sizes and polytypes, thus leading to an immense impact on the future optoelectronic nanodevices. According to the previous studies, there is no research concerning with the structural parameters consisting of shapes, sizes and geometric structures on the physical behaviors of SiC nanostructures. Hence in the present investigations, I mainly focus on the single-particle gaps, excitonic gaps and electron–hole interactions in SiC nanostructures with different sizes and shapes. In addition to the shapes and sizes, the incorporation of geometric structures is a common way to modify such physical properties of SiC nanostructures.

To determine the electronic structures of nanostructures, there are several theoretical methods such as the effective-mass approximation (EMA), the first-principle calculations and empirical models. EMA is only appropriate for comparatively large nanostructures. However, because of the presence of the non-parabolic dispersion in the band structure away from the center of the first Brillouin zone and the nonexistence of an atomistic description in the single-particle Hamiltonian, EMA is unsuccessful to study the physical properties of the small nanostructures. As a reason, the first-principle calculations [14–16] and empirical models [17–20] are beneficially proposed for the detailed studies. Owing to the high computational resource of the first-principle calculations, empirical models are widely exploited to study such nanostructures. Tight-binding and pseudo-potential methods are the attractive empirical models. Considering the atomistic wave functions, a tight-binding model [17,18] is described by a small basis set, while a pseudo-potential model [19,20] is defined with a large basis set. Due to the satisfied numerical requirement, the tight-binding theory is proposed to be implemented as an atomistic tool of the computations for the nanostructures.

This work is organized as follows: in Section 2, the theoretical frameworks I use are briefly described, while Section 3 is devoted to the discussion of the results concerning with the electronic properties of SiC nanostructures with different shapes, dimensions and geometric structures. The single-particle gaps, excitonic gaps and electron–hole interactions are analyzed. Finally, the conclusions are demonstrated in Section 4.

2. Theory and methodology

2.1. sp^3s^* Tight-binding method

The detailed computation begins with the zinc-blende and wurtzite atomic positions. Zinc-blende and wurtzite structure are built up from face-centered cubic lattice (FCC) with two atoms per unit cell and hexagonal closely packed lattice (HCP) with four atoms per unit cell, respectively. Nanostructures are chemically synthesized and the surface is passivated by organic ligands. Because of the flexible surrounding matrix, the nanostructures are nearly unstrained [21]. The atomic positions of the nanostructures are determined by cutting an arbitrary shape out of a bulk semiconductor without any surface relaxation impacts. The dangling bonds on the surface of the nanostructures are terminated by the procedure as described by Lee et al. [22] The single-particle states are written as a linear combination of atomistic orbitals α localized on each atom R with N_{at} being the total number of atoms in the system

$$\Psi(\vec{r}) = \sum_{R=1}^{N_{at}} \sum_{\alpha=1}^{10} C_{R,\alpha} q_{R,\alpha}(\vec{r} - \vec{R})$$

Table 1

Tight-binding parameters for SiC material [24]. a and c describe anion and cation. The subscripts s, p and s^* stand for s, p and s^* orbital, respectively. x and y are p_x and p_y orbital.

Parameters	Values (eV)
E_s^a	−8.4537
E_p^a	2.1234
E_s^c	−4.8463
E_p^c	4.3466
$E_{s^*}^a$	9.6534
$E_{s^*}^c$	9.3166
V_{ss}	−12.4197
V_{xx}	3.0380
V_{xy}	5.9216
$V_{sa,pc}$	9.4900
$V_{sc,pa}$	9.2007
$V_{s^*a,pc}$	8.7138
V_{pa,s^*c}	4.4051
Δ_a	0.0000
Δ_c	0.0585

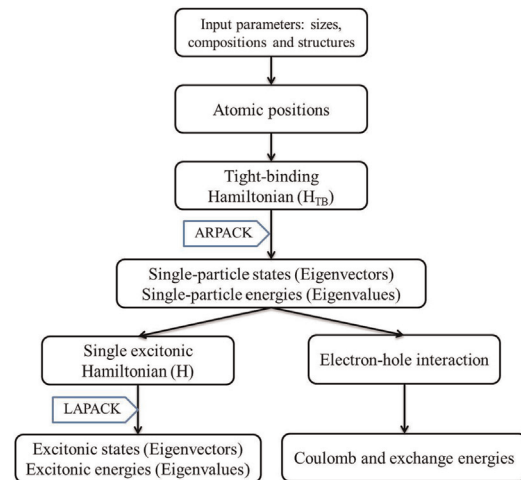


Fig. 1. The procedure of the model based on the atomistic tight-binding theory.

Table 2

The number of atoms in SiC nanocrystals with zinc-blende (ZB) and wurtzite (WZ) structure as a function of diameters (D_c).

Diameters (D_c) (nm)	Zinc-blende (ZB)	Wurtzite (WZ)
1.00	47	48
1.50	159	165
2.00	417	415
2.50	801	808
3.00	1363	1406
3.50	2149	2228
4.00	3193	3246

The coefficients $C_{R,\alpha}$ determine the i^{th} single-particle states and the single-particle energies. The empirical tight-binding Hamiltonian [23] is described by the operator $c_{R\alpha}^\dagger$ ($c_{R\alpha}$) creates (annihilates) the particle on the orbital α of atom R and is parameterized by the on-site orbital energies $\epsilon_{R\alpha}$, the spin–orbit coupling constant $\lambda_{R\alpha\alpha}$, and the hopping matrix elements $t_{R\alpha,R'\alpha'}$, connecting different orbitals situated at neighboring atoms:

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