Tight-binding description of the silicon carbide nanotubes

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Raad Chegel

Physics Department, Faculty of Science, Malayer University, Malayer, Iran

ABSTRACT

The electronic and optical properties of silicon carbide nanotubes (SiCNTs) have been investigated using tight binding calculations based on previous density functional theory (DFT) studies. The optical spectra of SiCNTs are dependent on the diameter and chirality and their energy gap (E_g) reduction shows dependence on radius and electric field. The E_g of SiCNTs decreases linearly with electric field until reaches zero and semiconductor metallic transition occurs. Based on the dependence of band gap reduction on radius and electric field strength, the E_g explained in terms of radius and electric field with an explicit relation.

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1. Introduction

One dimensional nanometer materials have attracted interest owing to their potential applications in the electronic, optoelectronic, and sensor devices. Silicon carbide nanotube (SiCNT) is a large band-gap material that can be a promising candidate for high chemical inertness, hardness, breakdown field and a electronic mobility [1]. Carbon nanotubes (CNTs) can be metallic or semiconductor depending on the way they are rolled up and their physical properties such as optical dielectric functions, depend sensitively on their chirality [2]. Beside CNTs, other tubular materials, such as BN [3,4], SiC [5,6] and GaN [7,8] have been predicted theoretically and detected experimentally and they have some very interesting properties distinctly different from their bulks. Unlike CNTs which are metallic or semiconductor, the SiCNTs are semiconductors similar to BNNTs [9]. The structure, electronic and optical properties of SiCNTs have been investigated based on the density functional theory [DFT] [9–12]. The adsorption of different molecules such as oxygen [13–15], CO [16,17] and NO [18] on SiCNTs have been investigated based on the DFT and it has been shown that SiCNTs can be potential efficient gas sensors for gas detection.

The electronic transport properties of SiCNT in presence of boron (B) nitrogen (N) impurities were investigated theoretically [19] and the results show that an energetically favorable configuration is obtained when B and N atoms located at neighboring Si and C

sites respectively [20]. Also it is found that the co-doping BN impurities suppresses the important negative differential resistance (NDR) property [21] and the conductivity of SiCNT reduces by increasing the BN dopant density [22]. The SiCNT with Fe dopant indicate the anti-ferromagnetism and ferromagnetism features when Fe substitutes Si and C, respectively [23]. The band structure and optical dielectric function of SiCNTs have been calculated within DFT and it is found that the SiCNTs in the low and high-energy region, exhibit broad peak at ~3 and ~7 eV, respectively [9]. The quasiparticle band gap of SiCNTs with different chiralities behave differently in terms of tube diameter due to the difference in the curvature-induced orbital rehybridization among the different chiral nanotubes [24]. The effect of tube size on optical properties of the SiCNTs have been investigated and it was shown that the optical spectra of SiCNTs dependent on the diameter and chirality and the red shifts or blue shifts occurred in their dielectric function with increasing tube diameter [11].

It has been pointed out that the electronic and optical properties of different nanotubes such as CNTs, BNNTs and SiCNTs can be modulated in the presence of external electric field [25–32]. Therefore by changing and controlling these properties, their application would be greatly extended. Engineering these properties can be achieved via other ways such as strain, doping and introducing defects. Some of these methods such as electric field directly modify the electronic structure and alter band gap but some of them reduce the band gap by creating separate levels inside the gap [33,34]. The electric field modifies the electronic properties of nanotubes and these modifications directly reflect in

the optical spectra. For BNNTs, it has been shown that the gap reduction increases with the diameter and it is independent of chirality. Many studies investigated the modifications of the electric structure of SiCNTs by electric field [25,29,35]. Alfieri et al. by DFT have investigated the band gap width of SiCNTs in electric field and found a decrease in the band gap width as a function of the electric field and nanotube diameter [29]. The electronic and optical properties of SiCNTs with the tight binding approximation have not been investigated in previous studies and in this study our goal is to investigate these effects. Our tight binding calculations are needed to understand the existing and future electronic and optical experiments especially in the electric field.

This paper is organized as follows. The theoretical approach and computational method are described In the Sec. 2. The electronic structure and dipole matrix elements are investigated in the Sec. 3. The optical absorption function are discussed in the Sec. 4. The effects of electric field are investigated in the Sec. 5.

2. Theoretical approach

A single wall SiCNT can be characterized by non-negative integer numbers (n,m) and the chiral vector and radius is defined by $\mathbf{C} = n\mathbf{a}_1 + m\mathbf{a}_2$ and $R = \frac{b_0}{2\pi}\sqrt{3(n^2 + m^2 + nm)}$ where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive lattice vectors of a SiC graphene sheet and b_0 is the Si−N bond length [2]. In the absence of electric field, the Hamiltonian is described as:

$$H = H_1 + H_2$$

$$H_1 = \sum_{\alpha,l} \varepsilon_\ell^{(0)}(\alpha) \big|\alpha, l\rangle\langle\alpha, l\big| \tag{1}$$

$$H_2 = \sum_{<\ell,\ell'>} \sum_{\alpha,\beta} t_{\ell\ell'}^{\alpha,\beta} \big|\alpha, l\rangle\langle\beta, l'\big|$$

where $|\alpha, \ell\rangle$ and $|\beta, \ell|\rangle$ refer to Si and C atoms in ℓ-th unit cell and $\varepsilon_\ell^{(0)}(\alpha)$ is the on-site energy for α atom at the unit cell ℓ due to the π atomic orbital. The $t_{\ell\ell'}^{\alpha,\beta}$ is the nearest neighbor hopping integral between α and β atoms in the unit cells ℓ and ℓ'. The coupling between two atoms on a similar site described by H_1, while the off-diagonal Hamiltonian elements H_2 represent coupling between two atoms in different sites.

The wave function of two dimensional graphene Ψ^l can be written as a sum of two Bloch function Φ_s, in the graphene sheet unit cell as $\Psi^s(k, r) = \sum_\alpha C_\alpha^l(k)\Phi_s(k, r)$, where s = c,v indicates the conduction and valence bands, α is the label for the Si and C atoms in the unit cell and $C_\alpha^l(k)$ is the equation coefficients. The Bloch wave function is expressed by a linear combination of atomic π orbital $\Phi_s = \frac{1}{N_0} \sum_{R_s} e^{i\vec{k}\cdot\vec{R}_s}\phi(r - R_s)$ where R_s is the position vector for the Si or C atoms and N_0 is the total number of unit cells in the lattice [36]. The band structure $E^s(k)$ and equation coefficients are found by solving the Sherodinger equation $H\Psi^s(k, r) = E^s(k)\Psi^s(k, r)$. Calculation of all the elements of SiC Hamiltonian matrix requires on-site and hopping parameters. In this study, the fitted on-site and hopping parameters obtained with the DFT calculation [9,11].

Using the dipole approximation, the interband optical matrix elements of possible transitions between an initial state in the valence band to a final state in the conduction band is given by $D_{v\to c} = \Psi^c(k, r)|\vec{\nabla}|\Psi^v(k, r)$ where $\vec{p} = -i\hbar\vec{\nabla}$ is the linear momentum operator [37]. Investigation of dipole matrix elements

requires electronic wave functions $\Psi^s(k,r)$ in the valence and conduction bands and also wave function coefficients $C_\alpha^l(k)$ and after performing algebraic calculations, the dipole matrix element is obtained as:

$$D\left(\vec{k}\right) = \sum_{\alpha,\beta}\sum_{b_l} C_\alpha^{c*}(k)C_\beta^v(k)\, e^{i\vec{k}\cdot\vec{b}_l} b_l\phi(r)|\mathrm{H}|\phi(r - b_l) \tag{2}$$

where b_l corresponds to the position vector of the Si (C) atoms to their C (Si) neighbors. For light polarization parallel to the tube axis, the optical transitions take place between subbands with the same angular momentum [36].

Applying the periodic boundary conditions in circumferential and the longitudinal directions leads to decomposing the wave vector **k** into a components parallel and perpendicular to the tube axis ($\mathbf{k}_T$ and $\mathbf{k}_C$) [38]:

$$\vec{k} = m\,\overrightarrow{K_1} + k_z\frac{\overrightarrow{K_2}}{K_2} \quad \left(m = 1, 2, ..., N \quad \left|k_z\right| \le \frac{\pi}{T}\right) \tag{3}$$

where $\overrightarrow{K_2}$ is the reciprocal lattice vector along the nanotube axis and $\overrightarrow{K_1}$ is the discrete wave vector in the circumferential direction. N is the number of hexagons in the nanotube unit cell and T is the translational vector of the nanotube. The optical absorption of the transverse dielectric function for incoming light with a frequency ω is obtained by Ref. [37]:

$$\alpha(\omega) \equiv \frac{1}{\omega}\sum_{\vec{k}}\left|D\left(\vec{k}\right)\right|^2 \frac{\gamma}{(\omega - \omega^{cv})^2 + \gamma^2} \tag{4}$$

where $\hbar\omega^{cv} = \hbar\omega^c - \hbar\omega^v$ is the energy difference between valence and conduction bands, γ is broadening parameter and $D(\vec{k})$ is the optical matrix element and it contains all selection rules.

3. Electronic structure and dipole matrix elements

The determination of the dispersion relations and band gap of the SiCNTs by tight binding method need to find onsite energies and hopping parameters. For this purpose we obtained the values of these parameters by fitting to DFT results. By using the DFT results, the on-site energies show radius dependence while is not yet available from experiment.

Our fitting method using the reported band gap in previous DFT calculations [9,11,39], shows that t = 1.8 eV and the onsite energies in terms of nanotube radius r are $\varepsilon_1 = -\varepsilon_2 = \Delta_0$ with $\Delta_0 = \lambda_1 r^v + \lambda_0$ where γ is -1.229 and λ_0, λ_1 are -4.26 and 1.369 eV, respectively. In the rest of this paper, we used these parameters.

The calculated band gap of several (n,0) zigzag SiCNTs [Z_n-SiCNTs] in terms of n is displayed in Fig. 1(a). It is observed that the band gap of Z_6-SiCNT is smaller than 1 eV in agreement with [9] and the band gap increases to 2.5 eV by increasing nanotube diameter as shown in Fig. 1 (a). For the Z_{10}-, Z_{13}-, Z_{14}-, Z_{20}-and Z_{24}-SiCNTs the calculated band gap are 1.709, 1.967, 2.034, 2.271 and 2.346 eV, respectively and for (8,4) and (10,4) chiral SiCNTs the calculated band gap is 1.867 and 1.967 eV, respectively which are in good agreement with the first-principles calculations [9,11,39].

We fitted E_g as a function of n^{-1} for all Z_n-SiCNTs as shown in Fig. 1 (b). It is found that the E_g is linearly proportional to the n^{-1} for large radius Z_n-SiCNTs which could be described by the analytical linear function $c_1 n^{c_2} + c_0$ where the constant coefficients $[c_0, c_1, c_2] = [2.73, -16.85, -1.198]$, respectively. To confirm the validity of the obtained analytical function, we applied it to the several SiCNTs. For example the band gap for Z_{10}-, Z_{11}-, Z_{12}-, Z_{13}-, Z_{14}-, Z_{20} and Z_{24}-SiCNTs are about 1.667, 1.784, 1.878, 1.957, 2.023, 2.2715