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The effects of boron doping on the optical absorption of carbon nanotubes

Hamed Rezania*

Department of Physics, Razi University, Kermanshah, Iran

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ABSTRACT

The frequency behavior of optical conductivity of (9,0) zigzag carbon nanotube doped with Boron atoms, as acceptor impurities, has been addressed. In the context of tight binding model Hamiltonian. In order to study of doping effects, we add a local energy term to original Hamiltonian of the clean system. This term presents the effect of scattering of electrons from impurities through carbon nanotube. Green's function of the disordered system is found using self-consistent Born approximation. Linear response is employed to calculate the optical conductivity of disordered carbon nanotube in terms of electronic Green's function. The effects of both dopant concentration and tube's diameter are investigated in details. The results show the optical conductivity is independent of boron concentrations in high frequency region. At low frequencies values, the increase of boron concentration leads to reduce optical absorption spectra. Moreover, optical conductivity gets the higher amounts at high frequency when the temperature raises.

1. Introduction

Carbon nanotubes (CNTs) have received an increasing amount of interest owing to their novel properties and potential applications in nanodevices [1]. These materials [1,2] has been formed from carbon atoms arranged on rolled honeycomb lattice as cylindrical structure with nanometer diameter and micrometer length. CNTs have been very widely studied ever since their discovery [1] on account of their unique electronic [3] and mechanical [4] properties, properties that vary with the symmetry and environment of the tubes [2]. One of the most fascinating aspects of nanotubes is that they exhibit either metallic or semiconducting electronic properties depending on their diameter and the atomic arrangement along their circumference [3,5]. It has been investigated the electronic structures of isolated single-wall nanotubes as well as bundled nanoropes. For isolated tubes it is believed that (n,n) armchair SWCNT are metallic, whereas (n,0) (zigzag) and (n,m) (chiral) tubes are semiconducting, most with a gap of 0.7 or so [5,6]. The deliberate introduction of defects and impurities (dopants) into carbon nanotube could offer a possible route to change and tune its electronic properties. The creation of new energy levels in the band gap with associated electronic states is an important step to make electronic devices. For instance, the intercalation of alkali metals into SWCNT has been shown to increase the conductivity [7].

Optical spectroscopic techniques are one promising avenue for identifying and probing the geometric structure of nanotubes. The careful investigation of the optical spectrum gives the geometric structure of individual nanotubes. The sensitive dependence of the low energy absorption spectrum on the diameter has been experimentally demonstrated by Kataura et al. [8]. Detailed ultraviolet spectroscopic experiments also clearly indicate that the spectrum depends strongly on tube diameter [9]. Experimentally, optical properties of CNT's have been studied by the optical ellipsometry [10], by the electron energy loss spectroscopy [11], by the reflectivity measurements [12], and also by the absorption experiments [13]. within a theoretical work based on density functional theory, It has been indicated that the absorption spectrum in the ultra violet region depends strongly not only on nanotube diameter but also on chiral index [14]. The electrical properties of carbon nanotubes can be controlled by impurity doping. Moreover, several applications of doped CNTs have been suggested such as field emission sources [15], sensors[16] and composites. Since nitrogen and boron have small atomic size compared to the carbon case, these elements are the most commonly used nanotube dopants because of reasonable probability to enter the nanotube lattice [17,18]. The introduction of these hetero atoms such as boron or nitrogen into CNTs offers the possibility of tailoring their structural and electronic properties of [19,20]. Such doping has already been achieved by a variety of techniques, including arc discharge [19], pyrolysis [21] and

* Tel.: +98 831 427 4569; fax: +98 831 427 4569.
E-mail address: rezania.hamed@gmail.com

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chemical vapor deposition [22]. Arc discharge method is performed in presence of $H_2 + B_2H_6$ and also by arc discharge of boron-stuffed graphite electrodes while nitrogen-doped was obtained by arc discharge in the presence of H_2 + *pyrdine* or H_2 + *ammonia*.

Electronic quantum transport has been investigated in boron and nitrogen doped carbon nanotubes in the context of tight binding model using *ab initio* calculations [23]. The spectroscopic studies and ultrafast pump-probe measurements of highly nitrogen doped multiwalled carbon nanotubes [24]. In this experimental work, the effects of nitrogen dopants on the carbon nanotube's optoelectronic properties have been investigated using ultrafast pump-probe experiments. A theoretical study of the optical conductivity of graphene beyond Dirac cone approximation with different kind of disorder as resonant impurities, random distribution of on-site potential or random renormalization of the nearest neighbor hopping parameter has been presented in details [25]. For a large enough concentration of resonant impurities, a new peak in the optical conductivity is found, associated to transitions between the midgap states and the Van Hove singularities of the main Π-band Also an extensive theoretical study on the electrical conductivity of monolayer disordered graphene using Green's function approach within Born approximation has been performed [26].

The goal of the present work is to sort out the effect of boron doping in the frequency dependence of optical conductivity of metallic zigzag CNT. In particular, we study the diameter and temperature dependence of the optical conductivity as a function of frequency using Green's function approach. We applied tight binding model Hamiltonian that on-site energy term is added to it in order to account the scattering of electrons from boron and nitrogen atoms. Linear response theory [27] has been applied to calculate the optical conductivity i.e. time ordered energy current correlation, in terms of Green's function of disordered system. Self-consistent Born approximation is used to make electronic self-energy whereby the Green's function of disordered system is found. In the last section we discuss and analyse our results to show how boron concentration and temperature as well as tube's diameter affect the optical transport of metallic zigzag CNT(9,0).

2. Model Hamiltonian and Green's function

The dynamics of π-orbitals electrons in the disordered carbon nanotube structure can be described in the context of random tight binding model Hamiltonian on the honeycomb lattices. In the nearest neighbor approximation, this model Hamiltonian (H) is expressed as

$$\begin{aligned} H &= H_{t.b} + H_{dis}, \\ H_{t.b.} &= -t\sum_{i,j,\alpha,\beta}(c^{\dagger}_{i,\alpha}c_{j,\beta} + h.c.), \\ H_{imp} &= \sum_{i,\alpha}(\epsilon_{i,\alpha} - \mu)c^{\dagger}_{i,\alpha}c_{i,\alpha}, \end{aligned} \tag{1}$$

$H_{t.b}$ is the tight binding part of electronic Hamiltonian on the honeycomb lattice atomic sites. The effect of disorder on the dynamics of π orbitals electrons can be studied by adding the local Hamiltonian term (H_{imp}) to the tight binding Hamiltonian. This term breaks the translational symmetry of crystal so that it introduces the scattering of electrons from impurities situated at randomly distributed but fixed positions. Since atomic number of boron atoms is fewer than that of carbon ones, the boron atoms as acceptor impurities play the role of quantum barrier in the scattering of electrons. In Eq. (1), t is hopping integral between nearest neighbors atoms belonging two sublattices A and $B(t \approx 2.7\,eV)$. $c_{i,\alpha}(c^{\dagger}_{i,\alpha})$ refers to the annihilation (creation) operators of electrons on the unit cell with position vector $\mathbf{R}_i$ and on the sublattice α. Also $\epsilon_{i,\alpha}$ is the strength of scattering random potential at sub-lattice α in the Bravais lattice unit cell $\mathbf{R}_i$. Half filling constraint corresponding to one electron per each lattice site implies chemical potential (μ) is to be zero. According to the crystal structure of honeycomb lattice in Fig. 1 the primitive unit cell vectors of honeycomb lattice including two triangular sublattices A, B has been described by the following

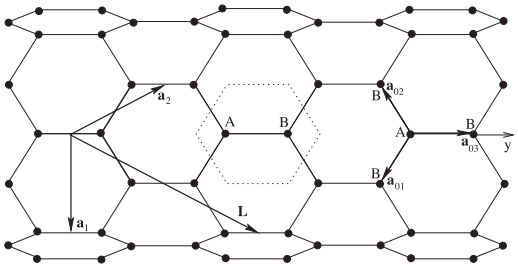

Fig. 1. A zigzag CNT whose axis is along the y axes. The light dashed lines denote the Bravais lattice unit cell. Each cell includes two nonequivalent sites, which are indicated by A and B. $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive vectors of unit cell. $\mathbf{a}_{01}$, $\mathbf{a}_{02}$ and $\mathbf{a}_{03}$ are three vectors that connect nearest neighbor sites.

$$a_1 = a\mathbf{i} \quad a_2 = \frac{1}{2}(-\mathbf{i} + \sqrt{3}\mathbf{j}), \tag{2}$$

where $\mathbf{i}$ and $\mathbf{j}$ are unit vectors along x and y directions, respectively. The axis direction of zigzag CNT is assumed to be along y direction. To determine the range of variation of wave vector, one should be noticed to the periodic boundary condition for CNT (m, n). In the x direction implies that $exp(ik_xL) = 1$ where and R denotes CNT's radius according to both boundary condition and Brillouin zonf of honeycomb lattice k_x is restricted to $k_x = 2\pi p/L = 2\pi p/a\sqrt{m^2 + n^2 + mn}$ where p, m and n are the integer numbers and $\mathbf{L}$ is the circumference of cross section of CNT [28]. In the following, the on-site energy of electrons in the presence of boron atoms takes the value 2.33 eV. Since honeycomb lattice is composed by two sublattice, the Green's function of the clean system can be written as the 2×2 matrix

$$\mathbf{G}(\mathbf{k}, i\omega_n) = \begin{pmatrix} G^{(0)AA}(\mathbf{k}, i\omega_n) & G^{(0)AB}(\mathbf{k}, i\omega_n) \\ G^{(0)BA}(\mathbf{k}, i\omega_n) & G^{(0)BB}(\mathbf{k}, i\omega_n) \end{pmatrix}. \tag{3}$$

In the Matsubara formalism [27], each element of the Green's function matrix and its Fourier transformation is defined by

$$\begin{aligned} G_{\alpha\beta}(\mathbf{k}, \tau) &= -\langle T_\tau c_{k,\alpha}(\tau)c^{\dagger}_{k,\beta}(0)\rangle \\ G_{\alpha\beta}(\mathbf{k}, i\omega_n) &= \int_0^{\beta} e^{i\omega_n\tau}G_{\alpha\beta}(\mathbf{k}, \tau)d\tau \end{aligned} \tag{4}$$

where α, β refer to each sublattice A or B and τ is the imaginary time. Also $\omega_n = (2n+1)\pi/\beta$ introduces Fermionic Matsubara's frequency. After performing a little algebraic calculation, Fourier transformation of the elements of Green's function of the clean system ($G^{(0)}$) can be obtained in the following forms

$$\begin{aligned} G^{(0)}_{AA}(k, i\omega_n) &= G_{BB}(k, i\omega_n) = \sum_{j=\pm}\frac{1}{4}\frac{1}{i\omega_n - E_j(k)}, \\ G^{(0)}_{AB}(k, i\omega_n) &= \sum_{j=\pm}\frac{1}{4}\frac{\phi^*(k)}{E_+(k)}\left(\frac{j}{i\omega_n - E_j(k)}\right), \\ G^{(0)}_{BA}(k, i\omega_n) &= \sum_{j=\pm}\frac{1}{4}\frac{\phi(k)}{E_+(k)}\left(\frac{j}{i\omega_n - E_j(k)}\right), \\ E_{\pm}(\mathbf{k}) &= \pm|\phi(k)|,\ \phi(k) = 1 + \cos(k_x/2)\exp(-ik_y\sqrt{3}/2). \end{aligned} \tag{5}$$