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Dependence of electron binding energies of semiconducting double walled carbon nanotube on magnetic field and inter-wall distance

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ABSTRACT

In this study the binding energies of semiconducting double walled carbon nanotube (DWCNT) were calculated using the variational method considering the effective mass approximation and confinement potential under external magnetic field. The study reveals that the 2p state splits into three states $2p^0$, $2p^+$ and $2p^-$. The binding energies of $2p^+$ and $2p^-$ states increases with increase in applied external magnetic field at a given inter-wall distance. Furthermore the binding energies of the states is found to decrease with increase in inter-wall distance and becomes appreciably small (<45 meV) for DWCNT with 0.42 nm inter-wall distance. In addition, our results reveal that for smaller core diameters the electron effective mass increases sharply and attain a peak value around at 0.2 nm and for large tube diameters (>0.8 nm), the electron effective mass becomes constant. The observed results were compared with the previously reported results.

1. Introduction

Carbon nanotubes (CNTs) are interesting nano-materials made exclusively of carbon atoms [1]. CNTs have astounding opto-electronic properties that arise due to low dimensional size particularly in nanometer range. These unique properties yield variety of promising applications such as CNT transistors, nano-sensing [2,3] etc. CNT is formed by wrapping one atomic thick layer of carbon called graphene which posses tubular morphology [4]. Generally CNTs can be categorized into two types, single walled nanotube (SWCNT) and multi-walled carbon nanotube (MWCNT). On the basis of electronic and vibrational properties, double walled carbon nanotubes (DWCNTs) are similar to those of SWCNTs, but they differ in their thermal and mechanical stress property [5]. The inner layer of DWCNTs can be approximated as an isolated SWCNT exhibiting rich variety of intriguing electronic properties and thus became promising material for electronic nano devices.

The electronic and optical properties of materials generally can be obtained by their quantum states. In nano based structures, these quantum states arise due to electron/hole confinement either in one or two dimensions. Thus DWCNTs are more prone for the fabrication of nano-devices, viz field emitters [6]. In this way, we need to understand the mechanism of the energy transfer between two inner and outer layers of DWCNTs to unveil their potential for future implications. Usually, the inner and the outer layers of DWCNTs possess the following four possible configurations: Metallic-Metallic, Metallic- Semiconducting, Semiconducting-Semiconducting, Semiconducting-Metallic. Each configuration is expected to possess distinct electronic properties [7]. Due to large electron confinement in the core regime of the DWCNT owing to the effect of presence of outer wall, large binding energies presume in the expected range of tens of MeV depending on tube diameter [8].

In this paper variational methods is used to calculate the electron binding energies of semiconducting DWCNT under the application of uniform external magnetic field within the effective approximation and confinement potential. Our theoretical results show that electron binding energy is dependent on both applied magnetic field and inter-wall distance. The possible reason for variation of binding energy with applied magnetic field at a constant inter-wall distance is also discussed.

The paper is organized as:

Section 2 describes the model and theoretical formulations and Section 3 presents the results and discussions. The conclusion remarks are presented in Section 4.

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2. Model and theoretical formulations

A theoretical model has been designed to calculate the electron binding energies of semiconducting DWCNT under the application of external magnetic field. In our model both inner and the outer tube is semiconducting in nature but differ in their band gaps, as the configuration is expected to possess distinct electronic properties. To infer the symmetric magnetic confinement in the x-y plane a uniform magnetic field is applied along z-direction.

The geometrical view of semiconducting DWCNT under consideration is shown in Fig. 1. Here a is the radius of the inner tube while b is the radius of the CNT as a whole, such that inter-wall distance is $t = (b - a)$.

The confinement potential is taken from the previously reported result [9], given by

$$V_e(r) = \frac{V_0}{a^2}\left(r^2 - a^2\right) \quad |r| \le a \tag{1}$$

Where V_0 is the conduction band offset potential between the two semiconducting layers of double walled carbon nanotube, which is equal to 0.4eV for a tube of diameter 1 nm [10].

The particle like electron experience strong confinement potential within the inner tube due to the presence of outer layer of the tube, in other words the particle experiences a strong confinement potential. Therefore the wave functions under such situations can exhibit Wentzel–Kramers–Brillouin (WKB) approximation [11], given by

$$\psi(a,b) = \begin{cases} \dfrac{A_s}{\sqrt{k_j}}\exp\left[-\displaystyle\int_a^b k_j dr\right] & For\ -b < r < -a \\ \dfrac{A_c}{\sqrt{k_j}} Sin\left[\displaystyle\int_{-a}^{a} k_j dr + \frac{\pi}{4}\right] & For\ -a < r < a \\ \dfrac{A_s}{\sqrt{k_j}}\exp\left[-\displaystyle\int_a^b k_j dr\right] & For\ a < r < b \end{cases} \tag{2}$$

Here j can be an electron (e) or a hole (h), A_c and A_s are the normalization constants of the inner core and outer shell of the DWCNT and the wave vector k_j is given by Ref. [10].

$$k_j = \frac{2n\pi}{\sqrt{3}a_{c-c}\sqrt{n^2 + mn + m^2}} \tag{3}$$

$$k_j = \frac{2n\pi}{8\sqrt{3}a_{c-c}} \quad \text{For semiconducting CNT} \tag{4}$$

where $a_{c-c} = 1.44A^0$ is the distance between the carbon atoms and n is an integer.

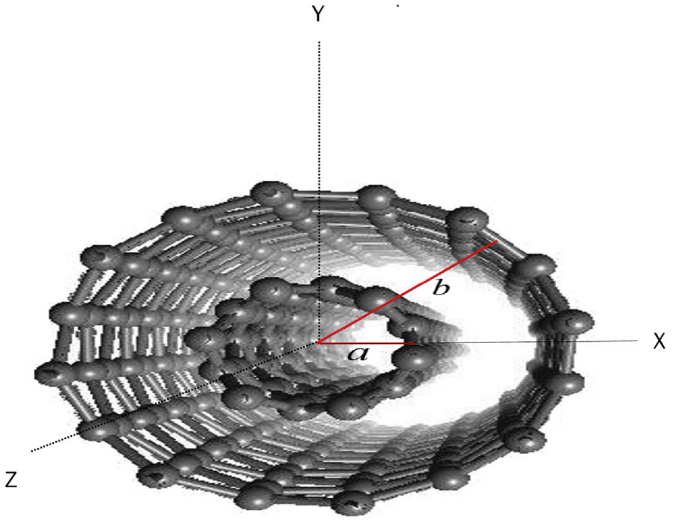

Fig. 1. Geometrical view of Semiconducting DWCNT.

Theoretical formulations

The Hamiltonian for a semiconducting DWCNT in the manifestation of magnetic field B taking into account the effective mass approximation and confinement potential is given by

$$H = \frac{1}{2m_e^*}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{e^2}{\varepsilon r^2} + V_e(r) + m_j g_e^* \mu_B B \tag{5}$$

Where m_e^* is the effective mass of the electron, g_e^* and μ_B are the effective g-factor for the electron and Bohr magnetron respectively. ε, e are dielectric constant electron and electron charge respectively. $\vec{A}$ is the vector potential of the magnetic field. In Equation (5), $H = \frac{1}{2m_e^*}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2$ represents the kinetic energy operator term, $-\frac{e^2}{\varepsilon r^2}$ represents the coulomb potential, $V_e(r)$ represents the confinement potential and $m_j g_e^* \mu_B B$ represents the Zeeman function.

The application of an external magnetic field restricts the motion of electron within the cyclotron radius $r_c = \sqrt{\frac{h}{2\pi e m_e^*}}$ [12] where h is planks constant. In the presence of magnetic field, the energy level in the plane perpendicular to the magnetic field gets quantized. It gives formation of degenerate energy levels. The binding energy under the influence of magnetic field is obtained as [13].

$$E_{binding} = \frac{\langle\psi|H|\psi\rangle}{\langle\psi\backslash\psi\rangle} \tag{6}$$

Where the Hamiltonian is given by Equation (5) and the wave function chosen is

$$\psi = \frac{A_s}{\sqrt{k_j}}\exp\left[-\int_a^b k_j dr\right] \quad For\ a < r < b \tag{7}$$

After various calculations, we obtained the final expression for binding energy for a semiconducting DWCNT as

$$E_{binding} = \frac{n^2h^2}{8m_e^*(t^2 + 2at)} - \frac{(t^2 + 2at).V_0}{a^2} + m_j g_e^* \mu_B B \tag{8}$$

3. Results and discussions

We calculated the electron binding energies of semiconducting DWCNT as a function of external magnetic field strength with certain inter-wall distance. The parameters chosen for numerical analysis are $m_e^* = 0.126m_o$, where m_o is the mass of free electron, conduction band offset potential $V_0 = 0.4eV$, lande-g factor for electron $g_e^* = 1.2$, carbon-carbon distance $a_{c-c} = 1.44A^0$ and $\mu_B = 9.27 \times 10^{-24}$ J/T.

The variation of binding energies of 2s and 2p excited states as a