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Electronic structures of double-layer zig-zag carbon nanotube

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Abstract. We study the electronic spectra of (9,0)-(18,0) double walled carbon nanotubes. We take into account the difference in Fermi levels of individual shells. As a result we get relatively small broadening of energy gap of double wall nanotube in comparison to the case with the absence of the intertube interaction.

1. Introduction

A single-wall carbon nanotube can be described as a graphene sheet rolled into a cylindrical shape so that the structure is one-dimensional with axial symmetry and in general exhibiting a spiral conformation called chirality. The primary symmetry classification of carbon nanotubes is as either being achiral (symmorphic) or chiral (non-symmorphic). Achiral carbon nanotubes are defined by a carbon nanotube whose mirror images have an identical structure to the original one. There are only two cases of achiral nanotubes, armchair and zigzag nanotubes. The names of armchair and zigzag nanotubes arise from the shape of the cross-section ring at the edge of the nanotubes. Chiral nanotubes exhibit a spiral symmetry whose mirror image cannot be superposed onto the original one. There is a variety of geometries in carbon nanotubes which can change the diameter, chirality and cap structures. The electronic structure of carbon nanotubes is derived by a simple tight-binding calculation for the π-electrons of carbon atoms. Of special interest is the prediction that the calculated electronic structure of a carbon nanotube can be either metallic or semiconducting, depending on its diameter and chirality. The energy gap for a semiconductor nanotube, which is inversely proportional to its diameters, can be directly observed by scanning tunneling microscopy measurements. The electronic structure of a single-wall nanotube can be obtained simply from that of two-dimensional graphite. By using periodic boundary conditions in the circumferential direction denoted by the chiral vector C_h, the wave vector associated with the C_h direction becomes quantized, while the wave vector associated with the direction of the translational vector T along the nanotube axis remains continuous for a nanotube of infinite length. Thus, the energy bands consist of a set of one-dimensional energy dispersion relations which are cross sections of those for two-dimensional graphite. To obtain explicit expressions for the dispersion relations, the simplest cases to consider are the nanotubes having the highest symmetry, e.g. highly symmetric achiral nanotubes. We are interested in this paper in the zigzag double-wall nanotubes(DWNs). We focus on $(9,0) - (18,0)$ zigzag

tubules. The synthesis of DWNs has been reported recently [1, 2]. Their electronic structure was investigated by the local density approximation [3, 4] and the tight-binding model [5, 6, 7, 8, 9].

2. $(9,0)-(18,0)$ zigzag tubules

To construct the Hamiltonian, we use only the valence and conductive states of individual nanotubes in the absence of intertube interaction. The electronic structures can be calculated from the Hamiltonian

$$H=\begin{pmatrix} \Delta+b2 & 0 & H_{3,11} & H_{3,12} \\ 0 & \Delta-b2 & H_{4,11} & H_{4,12} \\ H_{11,3} & H_{11,4} & -\Delta+b6 & 0 \\ H_{12,3} & H_{12,4} & 0 & -\Delta-b6 \end{pmatrix} \tag{1}$$

where

$$b2=\gamma_0(1-2\beta\cos\frac{\sqrt{3}ka}{2}+\beta^2)^{\frac{1}{2}}, \tag{2}$$

$$b6=\gamma_0(1-2\widetilde{\beta}\cos\frac{\sqrt{3}ka}{2}+\widetilde{\beta}^2)^{\frac{1}{2}}, \tag{3}$$

$$H_{3,11}=H_{4,12}=\frac{1}{4\sqrt{2}}\frac{\gamma_0}{8}\left(1+e^{-i(\varphi_6-\varphi_2)}\right), \tag{4}$$

$$H_{4,11}=H_{3,12}=\frac{1}{4\sqrt{2}}\frac{\gamma_0}{8}\left(1-e^{-i(\varphi_6-\varphi_2)}\right), \tag{5}$$

$$e^{i(\varphi_6-\varphi_2)}=\gamma_0^2\frac{1-\beta e^{i\frac{\sqrt{3}ka}{2}}-\widetilde{\beta}e^{-i\frac{\sqrt{3}ka}{2}}+\beta\widetilde{\beta}}{b2\ b6}. \tag{6}$$

$2\Delta(\approx\ 0.21eV)$ is a Fermi energy difference of the outer and inner nanotubes, $\Psi(k)=(d_3,d_4,d_{11},d_{12})$ and d_i is an amplitude to find electron in state ψ_i. The wave functions ψ_3,ψ_4 are conductance and valence states of outer nanotube and ψ_{11},ψ_{12} are conductance and valence states of inner nanotube in the absence of the intertube interaction [10]. The parameter $\gamma_0(\simeq 3eV)$ is the hoping integral in the graphene.

Since the radii of the outer and inner nanotubes are different $\beta\neq\widetilde{\beta}$. Here $k_y=k$ and $-\frac{\pi}{\sqrt{3}a}<k<\frac{\pi}{\sqrt{3}a}$ is a first Brillouin zone. As we have a curved surface, the local normals on the neighboring sites are no longer perfectly aligned and this misorientation also changes the transfer integral. The change can be calculated using the curvature tensor $b_{\alpha\beta}$ [11]. The result is

$$\frac{\delta t_a}{t}=-\frac{1}{2}b_{\gamma\beta}b^{\gamma}_{\alpha}\tau^{\beta}_a\tau^{\alpha}_a, \tag{7}$$

where only nonzero term is $b_{xx}b^x_x=1/R^2$. So we have

$$\frac{\delta t_1}{t}=0, \tag{8}$$

$$\frac{\delta t_2}{t}=-\frac{1}{2}b_{xx}b^x_x(\tau^x_2)^2=-\frac{1}{2R^2}(\tau^x_2)^2, \tag{9}$$

$$\frac{\delta t_3}{t}=-\frac{1}{2}b_{xx}b^x_x(\tau^x_3)^2=-\frac{1}{2R^2}(\tau^x_3)^2. \tag{10}$$

With using the unit vectors we have $(\tau^x_2)^2=(\tau^x_3)^2=\frac{a^2}{4}$. We found the radius of the inner nanotube from the expression $2\pi R=Na$. The nonzero terms are $\frac{\delta t_2}{t}=\frac{\delta t_3}{t}=\frac{1}{2}(\frac{\pi}{N})^2$. Similarly for the outer nanotube. The parameters β, $\widetilde{\beta}$ can be expressed in the form

$$\widetilde{\beta}=1-\frac{\delta t_2}{t}=1-\frac{1}{2}(\frac{\pi}{9})^2, \tag{11}$$

and

$$\beta = 1 - \frac{\delta t_2}{t} = 1 - \frac{1}{2}(\frac{\pi}{18})^2. \tag{12}$$

We assume the symmetric geometry of zig-zag DWN [7]. It was considered that hopping between shells takes place only between atoms which occupy position directly each above other. The eigenvalues of Hamiltonian (1) for some values of $\sqrt{3}ka/2$ near the point $k = 0$ are depicted on Fig.1. At the point $k = 0$ we get the wave function of the valence band in the form

$$\Psi_v \simeq -0.6\psi_3 + 0.8\psi_{11}. \tag{13}$$

We get the minimum gap $E_g = 0.09eV$ at the wave vectors $\sqrt{3}ka/2 \simeq \pm 0.05$. At these points the wave function of the valence band have the form

$$\Psi_v \simeq -0.263i\psi_3 + 0.838\psi_4 - (0.14 + 0.45i)\psi_{11} + (0.29 - 0.09i)\psi_{12}. \tag{14}$$

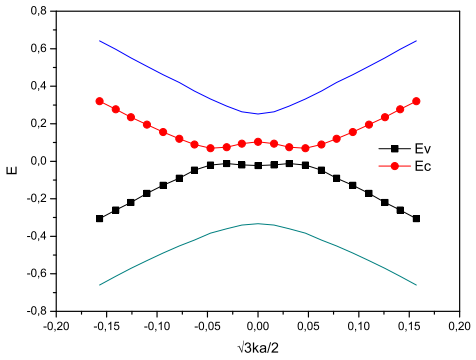

Figure 1. Spectra of zigzag DWN where E_c and E_v are conductive and valence band.

3. Conclusion

In the present work we take into account that the Fermi level of the individual nanotubes which create the double wall nanotubes are different. This difference is very important in the double wall nanotubes with small diameters. The interplay between energy difference of the Fermi levels of the individual nanotubes and the energy gaps between valence and conducting bands of individual nanotubes have a strong effect on the conductivity of double wall nanotubes [12, 13, 14, 15]. The important parameter is also a difference in the position of wave vectors k_F of individual nanotubes. The Fermi level of the outer shell is about 0.21 eV higher than the Fermi level of the inner shell in the case of zig-zag SWNs. In the case of zig-zag DWNs the curvature do not shift the k_F of the individual nanotubes. The result is that these DWNs are semiconductors.

Because of difference in Fermi levels of individual nanotubes the valence states are not symmetric to conduction states about the Fermi level in the absence of the intertube interaction. We have a gap $E_g = 25$ meV between the valence band of outer shell and the conductive band of inner shell. The difference in the Fermi levels of individual nanotubes have not been take into account in the work [7]. We get a minimum of the gap between valence and conductive band at a points $\sqrt{3}ka/2 \simeq \pm 0.05$ and a broadening of the energy gap $E_g = 90$ meV when the intertube interaction is imposed.

Generally we can say that the conductivity depends on the relative position of the Fermi points k_F of individual nanotubes. If there is no shift the DWN is a semiconductor. If there is a shift in the dependence on Fermi levels and the energy gaps of individual nanotubes the DWN can be semimetal or semiconductor.

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