Simulation the electronic properties of zigzag carbon nanotube(CNT)

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Abstract

In this paper, the energy dispersion relation has been calculated for zigzag carbon nanotubes to study their electronic properties and when they become metal or semiconductor depending on their diameters and chiral angles. The metal carbon nanotube was taken with chirality of (9,0), (12,0) and for the semiconductor carbon nanotube were (10,0), (13,0). The outcome gave various and tunable energy band-gaps.

Introduction

Carbon nanotubes can be thought of as graphitic sheets with hexagonal lattice that have been wrapped up into seamless cylinders. Since their discovery in 1991[1,2]. The carbon nanotubes provide extraordinary new properties which can be exploited for wide range new applications. These properties are not only limited to chemical properties but also in its electronic properties as well as mechanical properties[3]. The electronic properties of carbon nanotubes have attracted a lot of interest in both fundamental as well as application driven studies. Carbon nanotubes are predicted to be metallic or semiconducting depending on their diameter and the helicity of the arrangement of graphitic rings in their walls, so they depend on their chirality [4]. By depending on chirality, carbon nanotubes classified into three types namely, armchair (n,n) nanotubes, zigzag (n,0) nanotubes, and chiral (n,m) nanotubes, where n,m are integer values[5]. These tubes are called achiral nanotubes and the pictorial names come from observing the c-c bonding the tube's circumference. A nanotube is usually characterized by its diameter d_t and the chiral angle θ ($0 \leq |\theta| \leq 30°$). The chiral vector C_h is defined with the two integers (n, m) and the basis vectors of the graphene sheet

$C_h = na_1 + ma_2 \equiv (n, m)$ ....(1)

The chiral angle θ is the angle between the chiral vector Ch and the so-called "zigzag" direction (n, 0). The integers (n, m) determine dt and θ:[8]

$$d_t = \frac{a}{\pi}\sqrt{n^2 + m^2 + nm} \quad ....(2)$$

$$\sin\theta = \frac{m\sqrt{3}}{2\sqrt{n^2+m^2+nm}} \quad ...(3)$$

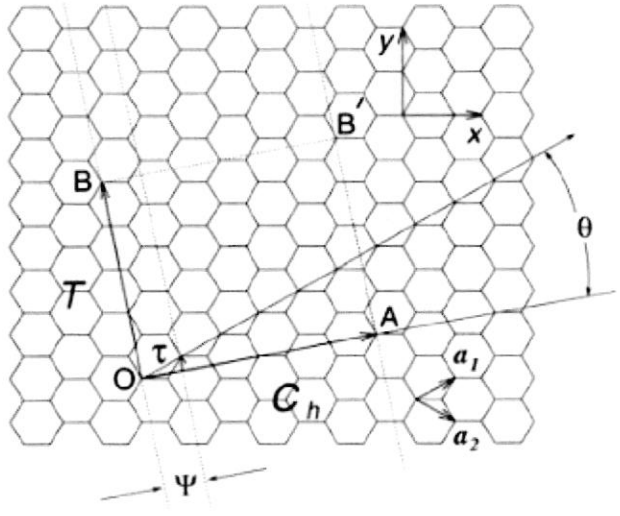

Fig.1: Definition of the unit cell of a carbon nanotube[9]

Theory

The essence of the various calculations of the 1D electronic band structure is based on a tight binding or Hiickel calculation that neglects curvature of the nanotubes [6]. Since atomic orbitals are mostly localized, the wave functions in the lattice can be represented by a linear combination of the mostly localized orbital of the atom. Taking into account two carbon atom basis of the lattice, the wave function may be modeled as:

$$\Psi_j(\vec{k},\vec{r}) = \sum_{j,j'=A,B} C_{jj'}\phi_{j'}(\vec{k},\vec{r}) \quad ...(4)$$

where $\phi_{A,B}$ are wave functions that satisfy Bloch equation[9]

$$\phi_{A,B}(\vec{k},\vec{r}) = \frac{1}{\sqrt{N_{A,B}}}\Sigma_{\vec{R}} e^{i\vec{k}}\varphi(\vec{r} - \vec{R}_{A,B}) \quad ....(5)$$

φ are the waveforms of the atomic carbon orbital and carbon coordinates, $\vec{R}_A$ and $\vec{R}_B$ are basis atom positions translated through the lattice. The based on Schrödinger equation solution for energies and

coefficients that determine the wave function comes by solving the coefficient equation:

$$[H - ES]C = 0 \quad \ldots(6)$$

H is the Hamiltonian which is given by

$$H_{jj'} = \langle \psi_j | H | \psi_{j'} \rangle \; ; \; S_{jj'} = \langle \psi_j | \psi_{j'} \rangle (j, j' = A, B) \quad \ldots(7)$$

are transfer and overlap integrals.Because we have identical atoms in the basis set, we can take

$$H_{AA} = H_{BB} = 0 \quad \ldots(8)$$

and

$$H_{AB} = H^{*}_{BA} = t.f(\vec{k}) = t(e^{ik_x a/\sqrt{3}} + e^{ik_x a/\sqrt{3}} \cos(k_y a/\sqrt{2})) \quad \ldots(9)$$

where k_x, k_y is the wave vector along the direction of carbon nanotube axes. The transfer integral between the two neighboring atomic orbital is given by value t:

$$t = \langle \psi_A | H | \psi_B \rangle \quad \ldots(10)$$

the basic approximation takes into account the nearest three atoms for the overlap since it is assumed that atomic orbitals are well localized. The energy dispersion relation is obtained by [7]

$$E(k_x, k_y) = \mp t \left[1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right) \right]^{\frac{1}{2}} \quad .(11)$$

where a is the lattice constant, which is the nearest-neighbor distance between any two atoms of carbon in the graphene sheet (a=1.421Å)[10] .

Results and discussion:

the simulation results for energy dispersion relation for zig-zag carbon nanotube of (9,0),(12,0) for metallic carbon nanotube are shown in fig(2) and fig(3). It is clear that the conductance and valance energy bands of graphene are degenerate by symmetry due to the crossing point (k)of the lowest conductance and highest valance subband of metallic carbon nanotube.

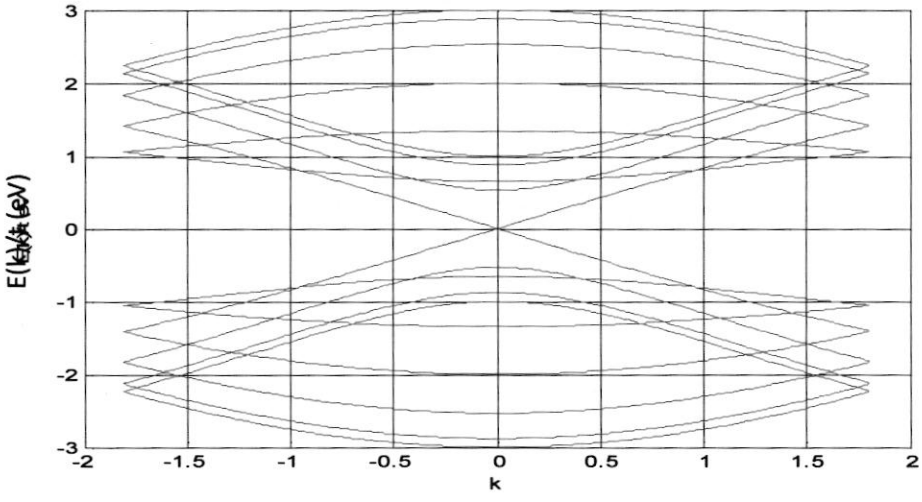

Fig.(2) One-dimensional energy dispersion relations for zigzag (9,0) metallic carbon nanotube.

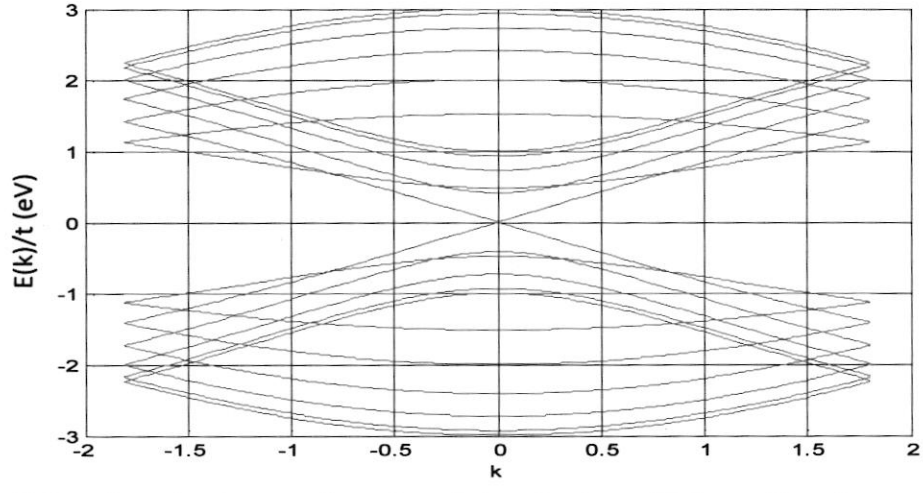

Fig.(3) One-dimensional energy dispersion relations for zigzag (12,0) metallic carbon nanotube.

The semiconducting behavior of zig-zag carbon nanotube are shown in fig(4) and fig(5) with chirality of (10,0), (13,0), respectively. The crossing sectional line in this case(i.e semiconducting behavior) does not pass through a (k) point.

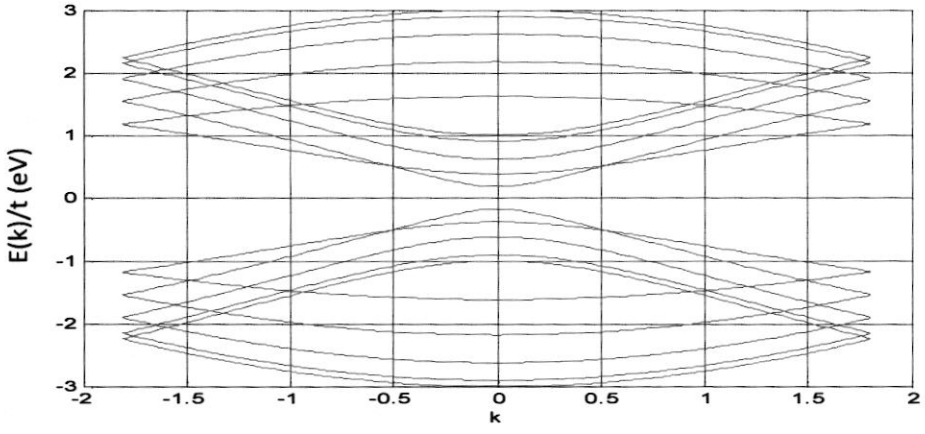

Fig.(4) One-dimensional energy dispersion relations for zigzag (10,0) semiconducting carbon nanotube

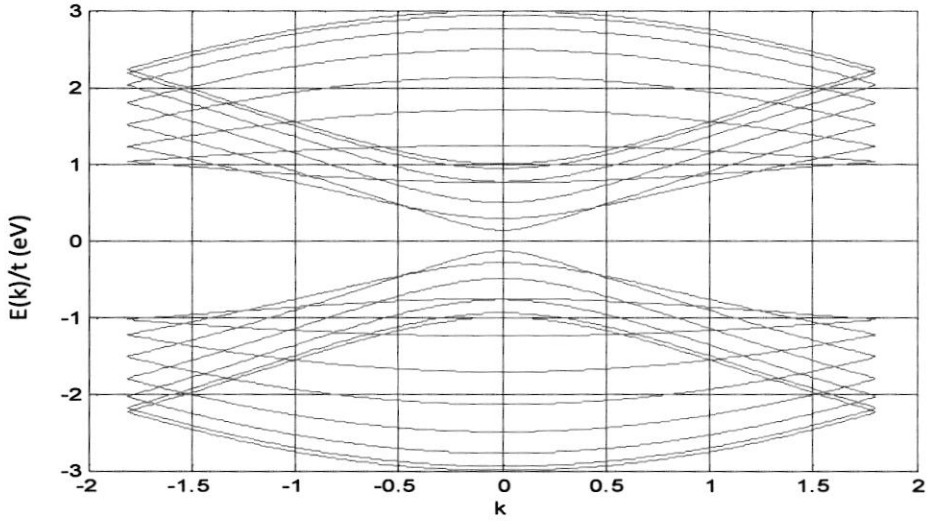

Fig.(5) One-dimensional energy dispersion relations for zigzag (13,0) semiconducting carbon nanotube

1D electronic structure shows that about third of carbon nanotubes are metallic by satisfying the metallic condition in general of carbon nanotube

$2n+m=3q$..... (12)

Where (n,m) are pairs of integers which is the chirality of carbon nanotube, q is integers. So for semiconducting it is not satisfied the above condition $(n-m\neq 3q)$.

The energy band-gap for carbon nanotube can be explained by [10]

$$E_g = \frac{t\, a_{c-c}}{d_t} \quad \text{..... (13)}$$

Theoretically the band-gap for semiconducting carbon nanotubes with a chirality (n,0) is inversely proportional to the diameter.

As shown in fig(6), for metallic, the mixing of the π/σ bonding and π^*/σ^* antibonding causes the band crossing (k_F) of graphene to shift away from the (k) point and produce small gaps, this small gap is negligible for nanotubes with large diameters.

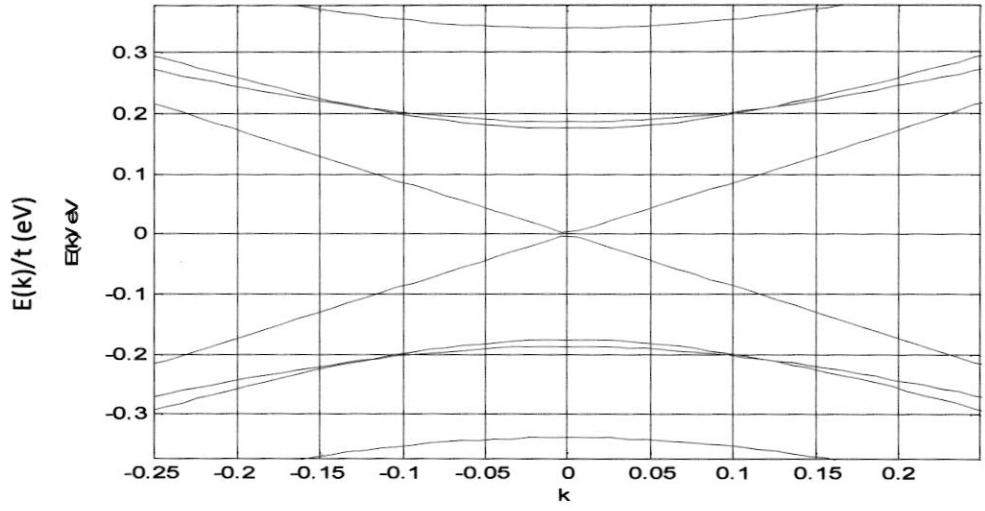

Fig.(6) One-dimensional energy dispersion relations for zigzag(30,0) metallic carbon nanotube.

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محاكاة الخصائص الالكترونية لانبوب الكاربون النانوي نوع المتعرج

هبة حسن عبدالله

قسم هندسة الليزر والبصريات ، الجامعة التكنولوجية ، بغداد ، العراق

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الملخص

في هذا البحث، تم حساب علاقة الطاقة المشتتة لأنبوب الكاربون النانوي نوع المتعرج ودراسة الخصائص الالكترونية في حالة كونه موصل او شبه موصل بالاعتماد على قطر الانبوب وزاوية chiral. انبوب الكاربون النانوي الموصل اخذ بالاعتماد على chirality (9,0)، (12,0) وللانبوب شبه الموصل اخذت chirality (10,0)، (13,0) .