

One Dimensional Tight Binding Computations for CNT Type, Diameters and Chirality at (1550, 1300)nm Communication Window Wavelength

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Abstract

In this paper, the electronic density of state (DOS) of a carbon nanotube has been calculated using Tight Binding (TB) method. The result based on the graphene sheet model, is deduced as a function of the nanotube chirality and diameter. These two latter properties in turn decide whether the CNT is metallic or semiconducting. The diameters for zigzag and armchair type of CNT were calculated according to energy gaps of (0.773), (0.922)eV the equivalent of 1550nm and 1300nm wavelength. The DOS of these energy gaps was simulated with the first energy level (E_{11}) using MATLAB.

Keywords: Carbon nanotubes, chirality, tight binding method, density of state.

الخلاصة

في هذا البحث، تم حساب كثافة الحالة الإلكترونية لأنبوب الكربون النانوي باستخدام طريقة (Tight Binding). النتائج المعتمدة على نموذج لوح الكرافين مستخلصة كدالة القطر و chirality لأنبوب الكربون النانوي. هذه الخاصيتين الأخيرتين بدورهما يقرران إما أنبوب الكربون النانوي معدني أو شبه موصل. تم حساب الأقطار للأنابيب النانوية نوع المتعرج والكرسي بالاعتماد على فجوات الطاقة (0.773، 0.922)eV ما يعادل (1550، 1300)nm طول موجي. تم محاكاة كثافة الحالة الإلكترونية لفجوات الطاقة مع مستوى الطاقة الأول E_{11} باستخدام MATLAB.

الكلمات المفتاحية: أنبوب الكربون النانوي، chirality، طريقة tight binding، كثافة الحالة.

Introduction

Since the discovery of carbon nanotubes (CNT) in 1991[S. Iijima, 1991], they have increasingly become very interesting worldwide because of their unusual properties and great potentials in technological applications. One of these applications is in optical communication, by making (CNT) as fiber and transmitting information with the most popular wavelengths in optical communication namely (1550 and 1300)nm. In this study, the (CNTs) have been taken as zigzag and armchair types. The electronic properties of CNT are of considerable interest which can exhibit either metallic or semiconducting behavior depending on their diameter and chirality[G.Y.Guo and K.C.Chu, 2004]. The electronic spectrum of metallic or semiconducting carbon nanotubes is characterized by a set of Van Hove Singularities (VHSs) that reflects the quantized number of the available electronic states. The Van Hove Singularities of the density of state (DOS) is of a great importance for many physical phenomena like conductivity and optical emission[S. Hugel, April 2003].

Theory

The electronic structure of a carbon nanotube consists of two-dimension graphene sheet as shown in Figure(1).

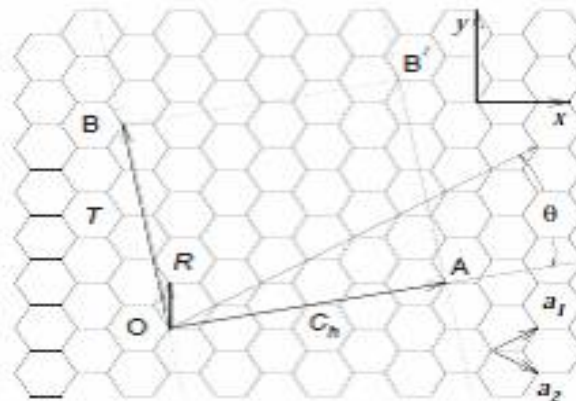


Fig.(1):Part of the graphene lattice[Saito, R., Dresselhaus,G. & Dresselhaus, M.S., 1998].

The chiral vector is [J. Karamdel, M. Damghanian, & F. Razaghian, 2010];

$$C_h = na_1 + ma_2; \quad (1)$$

where a_1 and a_2 are the graphene primitive vectors and n, m are integers. T in fig (1), defined as the translation vector, is directed along the CNT axis and perpendicular to C_h . The magnitude of T corresponds to the length of the (n, m) CNT unit cell [J. Karamdel, M. Damghanian, & F. Razaghian, 2010]. Once (n, m) is specified, other structural properties, such as diameter (d_t) and chiral angle (θ), can be determined as [Dresselhaus, G. & Dresselhaus, M.S., 1996];

$$d_t = (3^{1/2}/\pi)a_{cc}(m^2 + mn + n^2)^{1/2}, \quad (2)$$

$$\theta = \tan^{-1}[3^{1/2}m/(2n + m)], \quad (3)$$

where a_{cc} is the nearest-neighbor carbon atom distance. Those that are termed “zigzag”, “armchair” and “chiral” are designated by $(n, 0)$, (n, n) , and (n, m) respectively [J.G. Wildoer *et al.*, January 1998].

The calculations of the one dimensional (1D) electronic band structure is based on a tight binding calculation that neglects curvature of the nanotubes and satisfies the Schrödinger equation as [S. Z. Bisri, Sukirno & Irmelia, , 2009];

$$[H - E_i(\vec{k})S]C_i = 0 \quad (4)$$

where H and S are called transfer integral matrices and overlap integral matrices respectively.

The solution of Schrödinger equation belongs to differential equations and they must obey Bloch's theorem [S. Z. Bisri, Sukirno & Irmelia, , 2009];

$$\Psi_i(\vec{k}) = e^{(i\vec{k}\vec{r})}C_i(\vec{k})\Psi_i(\vec{k}) = e^{(i\vec{k}\vec{r})}C_i(\vec{k}) \quad (5)$$

This equation represents the periodic Bloch equation. $\Psi_i(\vec{k})$ are eigenfunctions for the conduction (valance) energy bands which can be expanded in Bloch orbitals $\Phi_i(\vec{k}, \vec{r})$ of "graphene unit cell" as;

$$\Psi_i(\vec{k}, \vec{r}) = \sum_{i \neq 1}^n C_{ii}(\vec{k}) \Phi_i(\vec{k}, \vec{r}) \Psi_i(\vec{k}, \vec{r}) = \sum_{i \neq 1}^n C_{ii}(\vec{k}) \Phi_i(\vec{k}, \vec{r}) \quad (6)$$

where n is the number of Bloch function. $C_{ii}(k)$ is the Bloch function coefficients.

The energy eigenvalues of eigenfunction states can be deduced as [S. Z. Bisri, Sukimo & Irmelia, 2009];

$$E_i(\vec{k}, \vec{r}) = \frac{\langle \Psi_i | H | \Psi_i \rangle}{\langle \Psi_i | \Psi_i \rangle} E_i(\vec{k}, \vec{r}) = \frac{\langle \Psi_i | H | \Psi_i \rangle}{\langle \Psi_i | \Psi_i \rangle} \quad (7)$$

From the above equation, the energy eigenvalues can be derived which are obtained as function of the wavenumber $\vec{k}$. Thus the energy dispersion relation may be derived to be [G. Ostojic, January 2005];

$$E(k_x, k_y) = \pm V_{pp\pi} \left[1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right) \right]^{\frac{1}{2}}$$

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The Density Of State:

It is possible to derive the DOS using a simplified expression for the graphene $E(k_x, k_y)$ that allows a completely analytic expression of the DOS for any CNT geometry as [J.W. Mintmire & White C.T., 1998];

$$n(E) = \frac{2\sqrt{3}}{\pi^2} \frac{1}{|V_{pp\pi}|} \frac{a_{cc}}{r} \sum_{\eta=-\infty}^{\infty} g(E, \varepsilon_{\eta}) n(E) = \frac{2\sqrt{3}}{\pi^2} \frac{1}{|V_{pp\pi}|} \frac{a_{cc}}{r} \sum_{\eta=-\infty}^{\infty} g(E, \varepsilon_{\eta}) \quad (9)$$

where

$$g(E, \varepsilon_{\eta}) = \begin{cases} \frac{|E|}{\sqrt{E^2 - \varepsilon_{\eta}^2}}, & |E| > |\varepsilon_{\eta}| \\ 0, & |E| < |\varepsilon_{\eta}| \end{cases}$$

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and $V_{pp\pi}$ is equal to the transfer integral, r is the radius of the nanotube and a_{cc} is the nearest neighbor distance between carbon atoms. The ε_{η} is the energy from wave vector component which is given by [J.W. Mintmire & White C.T., 1998];

$$|\varepsilon_{\eta}| = \frac{|3\eta - n + m|}{2} |V_{pp\pi}| \frac{a_{cc}}{r} |\varepsilon_{\eta}| = \frac{|3\eta - n + m|}{2} |V_{pp\pi}| \frac{a_{cc}}{r} \quad (11)$$

with n and m are integers which denote the chiral vector of the given nanotube.

Results and discussion

Energy dispersion relation for CNT

By taking different chiralities, a CNT can be deduced to be either metallic or semiconductor. Although there is no difference in chemical bonding between carbon atoms and there are no doping impurities in the CNT, it can behave as metal for all armchair and for zigzag when $(n-m)$ is a multiple of 3. Otherwise it behave as semiconductor. the energy dispersion relation was calculated using MATLAB to give indication if CNT is metallic or semiconducting. The energy dispersion relation for zigzag CNT with chirality (66,0) and for armchair with chirality (38,38), give indication

that CNT with these chiralities behave as metallic as shown in fig.(2), fig.(4). From fig(3) shows that the energy dispersion relation of zigzag CNT behave as semiconductor.

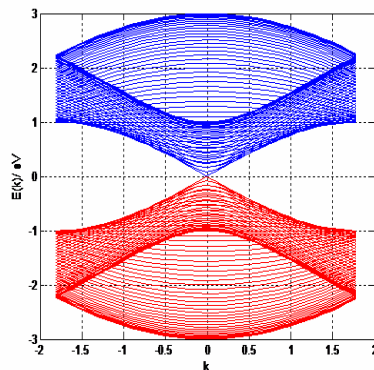


fig.(2) Energy dispersion relation for zigzag CNT (66,0).

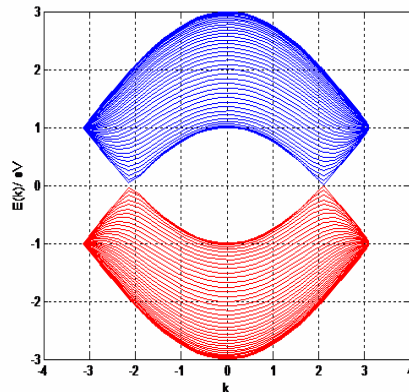


fig.(3) Energy dispersion relation for armchair CNT (38,38).

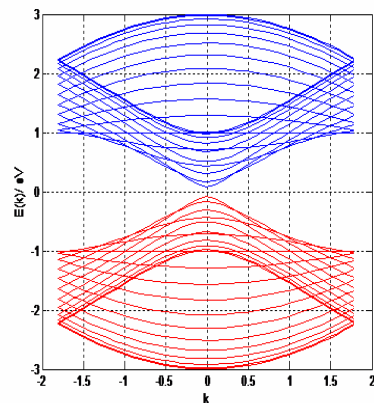


fig.(4) Energy dispersion relation for zigzag CNT (66,0).

Density of state for CNT

The (DOS) for the selective chirality of CNT was computed using MATLAB program. The DOS for semiconductor and metallic zigzag CNT with chiralities (22,0), and (66,0) respectively, are shown in fig.(5) and fig.(7), respectively. The DOS for armchair is shown in fig.(6) with chirality (38,38) referring to the wavelength (1550)nm.

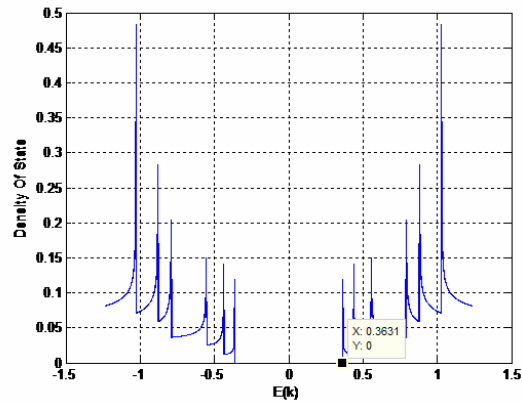


Fig.(5) The DOS for zigzag CNT (22,0)

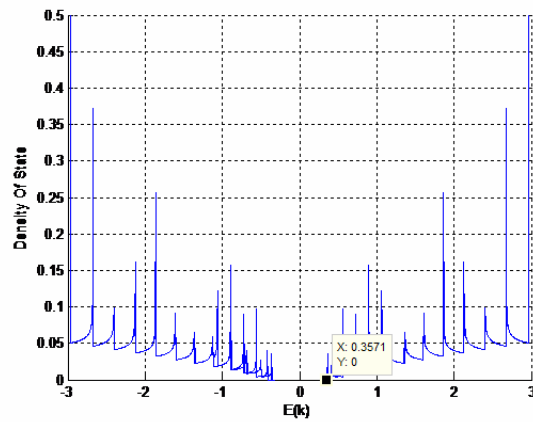
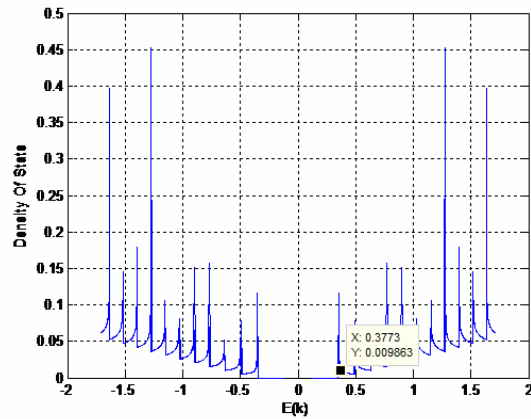


Fig.(6) The DOS for armchair CNT (38,38)



Fig(7) The DOS for zigzag CNT (66,0)

For (1300)nm wavelength, the DOS was calculated for semiconductor (19,0), metallic (54,0) zigzag CNT as shown in fig.(8) and fig (10), respectively. The armchair CNT with (32,32) chirality is shown in fig.(9).The energy band gap was calculated for these specific wavelengths as shown in Table (1) for (1550)nm and (1300)nm.

From the known wavelength (λ) the energy band gap can be calculated as[Sergei M. *et al.*, 2002];

$$E_g^s = 2\gamma_o a_{co} / d_t \quad (12)$$

$E_g^m = 6\gamma_0 a_{cc}/d_t$ (13)
 where E_g^s and E_g^m are the energy band gap for semiconductor and metallic CNT respectively.

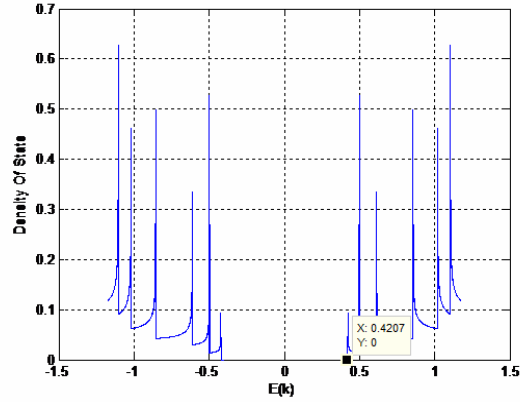


Fig.(8) The DOS for zigzag CNT (19,0)

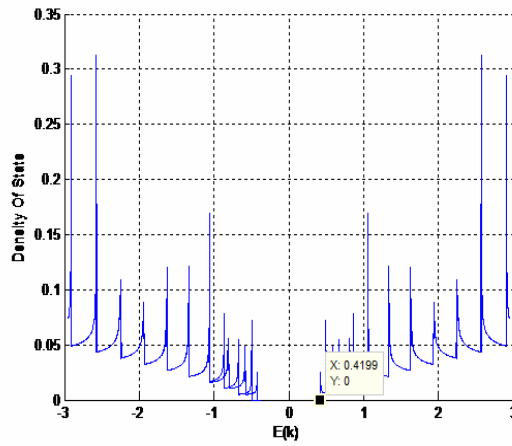


Fig.(9) The DOS for armchair CNT (32,32)

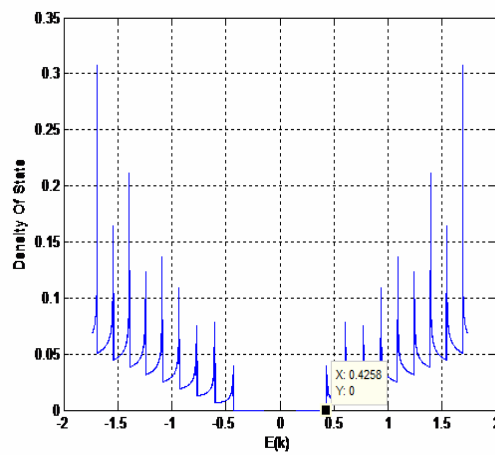


Fig.(10) The DOS for zigzag CNT (54,0)

Table (1)

Metallic CNT			Semiconductor CNT			
Chirality zigzag	Chirality armchair	$d_t(\text{nm})$	Chirality zigzag	$d_t(\text{nm})$	$E_g(\text{eV})$	$\lambda (\text{nm})$
(66,0)	(38,38)	5.135	(22,0)	1.718	0.773	1550
(54,0)	(32,32)	4.304	(19,0)	1.435	0.922	1300

By comparing with A. Hartschunh et al., they considered the SWNT structure with chiral type. The optical transition energies for specific wavelengths (881-1023)nm were calculated with chiralities (6,4)-(7,5). Single wall nanotube (SWNT) with these chiralities provide a stable, single molecule infrared photon source, with an extremely narrow linewidth, which would have a significant impact for future nanometer scale integrated photonic devices and which shows promise for applications in quantum optics and biological sensing.

Conclusion

In the present work, we conclude based on one dimensional tight binding (TB) theory, that for the interesting (1300,1550)nm wavelength for communication community carbon nanotube with armchair (32,32), (38,38) and zigzag (22,0), (19,0) are good source for those wavelength.

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