Mechanical Deformation Effect
to the Band Gap of Semiconducting Carbon Nanotube

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Abstract

The mechanical deformation effect of semiconducting carbon nanotube has an attractive property to be investigated. Recently, several researchers have thought to utilize this effect, because it has one advantage that it can be applied to develop electro mechanical devices. Using Tight Binding method, the mechanical deformation effect on the electronic properties of semiconducting nanotube has been investigated. We analyzed four semiconducting carbon nanotubes that are zig-zag and chiral CNT{ (8,0), (7,3), (7,2) and (6,4)}. The band gap of these semiconducting CNT decrease leading to a semiconductor-metal transition. However, further changes in deformation can increase the band gap that causes a metal-semiconductor transition.

Keywords: Mechanical deformation, Semiconductor-Metal transition, Metal-Semiconductor transition.

1. Introduction

Single-walled carbon nanotubes (SWCNT) is one dimensional structure composed of a one-atom-thick layer of rolled graphite sheets which form cylindrical tube[1]. CNT has recently attract a lot of attention in both experimental and theoretical research due to its unique physical properties (e.g. electronic and mechanical properties). The electronic structure of CNT is either metallic or semiconducting, depending on its diameter and chirality. The electrical and mechanical properties make it as a promising material for technological applications like nanosensor, switching devices, etc[2].

Recently, the deformation effect to the CNT band gap has been a topic of intense investigation. Based on the experimental results, the cross section of a carbon nanotube might be flattened/deformed for a large volume reduction in bundles of SWCNTs in high-presure experiment[3]. A recent experiment has shown that mechanical deformation can significantly change CNTs electronic behavior. It shows that the conductance of a metallic CNT can be reduced by two orders of magnitude through AFM tip-induced deformation[4]. Bogar.F, et al have studied the mechanical and electronic properties of several CNTs {(3,0), (4,0), (5,0), (6,0), (3,3), (4,4), (5,5), (6,6)} under axial stress. They found that the change of the band gaps because of applying small (< 5%) deformations results in semiconductor-metal transitions[5]. Using density functional theory (DFT), Peng.S, et al have also investigated the deformation effect to the zig-zag carbon nanotube (8,0). The band gap of this CNT showed the metal-semiconductor transition[6]. Yang Liu, et al also calculated and simulated the change of CNT band gap because of strain effect[7]. To show the deformation effect to the CNT band gap, Kleiner.A, et al have derived an analytic expression for these gaps[8].

In this paper, we explore the mechanical deformation on several semiconducting CNTs. We focus on {(8,0), (7,3), (7,2), (6,4)} CNTs because of two reasons. First, several researchers have just analyzed these effects on CNT just in general. The second reason is to compare the deformation effect to their band gaps in details.

2. Computational Details

In order to analyze and simulate the band gaps due to the deformation effect, we use several equations based on the tight binding method. The first equation is[9]

$$E(k) = \pm\gamma \left[\begin{array}{c} 1 + 4\cos\left(\frac{3C_x ka}{2C} - \frac{3\pi pa C_y}{C^2}\right)\cos\left(\frac{\sqrt{3}C_y ka}{2C} + \frac{\sqrt{3}\pi pa C_x}{C^2}\right) \\ + 4\cos^2\left(\frac{\sqrt{3}C_y ka}{2C} + \frac{\sqrt{3}\pi pa C_x}{C^2}\right) \end{array} \right]^{1/2} \quad (1)$$

where $C_x = a(\sqrt{3}n + (\sqrt{3}/2)m)$, $C_y = a(3/2)m$, $C = \sqrt{3}a\sqrt{n^2 + m^2 + nm}$, $a = 1.44\text{A}^0$, $p = 1...2n$, n and m are integers, and $\gamma = 2.5$ eV. The equation (1) is used to describe the relation between energy dispersion $E(k)$ and k. To estimate the deformation effect, we modify the equation (1) according to the equation (2)and the equation is[7]

$$E(k) = \pm t_2 \left[1 \pm \left(\frac{4t_1}{t_2}\right)\cos\left(\frac{\pi q}{n}\right)\cos\left((1+e)\frac{\sqrt{3}ka}{2}\right) + \left(\frac{2t_1}{t_2}\right)^2 \cos^2\left(\frac{\pi q}{n}\right) \right]^{1/2} \quad (2)$$

$t_2 = \gamma$, e is deformation parameter, $q = p$, and t_1 is related to the values of e. Using the equation that it has been derived by Kleiner.A, et al, we calculated the band gap of these carbon nanotubes. In our computation, we neglect the part of twist effect and we just use the uniaxial deformation. According to

that equation, the twist effect is suitable for armchair carbon nanotubes. The third equation is[8]

$$E_g = \left| \left(\frac{\gamma \pi^2}{8 c_h^5} - \frac{ab\sqrt{3}}{4 c_h^3} \varepsilon \right)(n-m)(2n^2 + 5nm + 2m^2) \right|$$

(3)

Where $c_h = C$, $\varepsilon = e$, and $b = 3.5$ eV.

We have chosen (8,0) semiconducting zig-zag tube, (7,3), (7,2) and (6,4) semiconducting chiral tubes for our study. All these tubes have nearly the same diameter of 6 A^0.

3. Results and Discussions

The dependence of the energy gap on the deformation effect is shown in figure1 and 2.
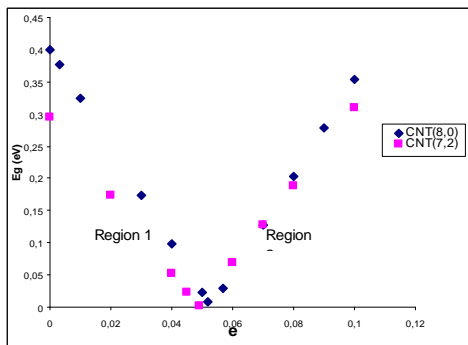
Fig.1. Energy gap as function of the deformation parameter of (8,0) and (7,2) carbon nanotubes.
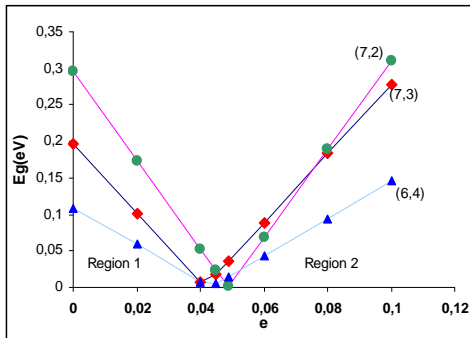

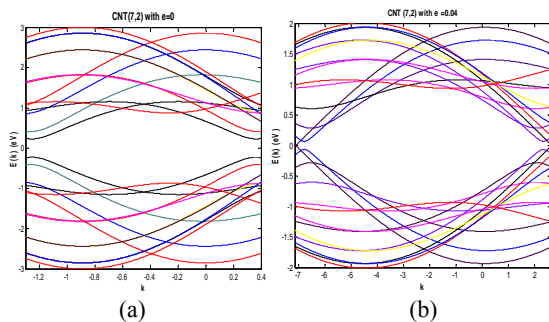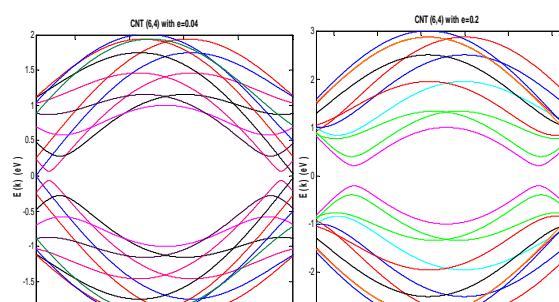Fig.2. Energy gap as function of the deformation parameter of (7,3), (7,2), and (6,4) carbon nanotubes.
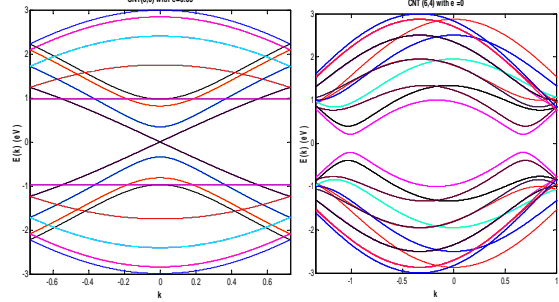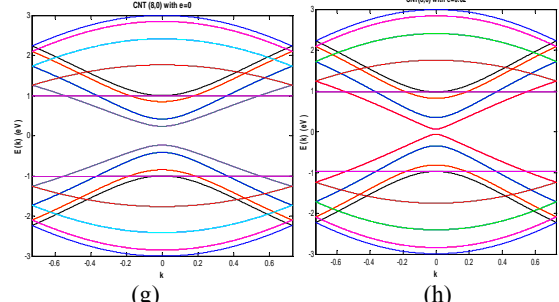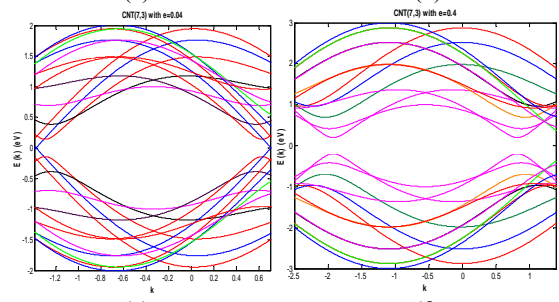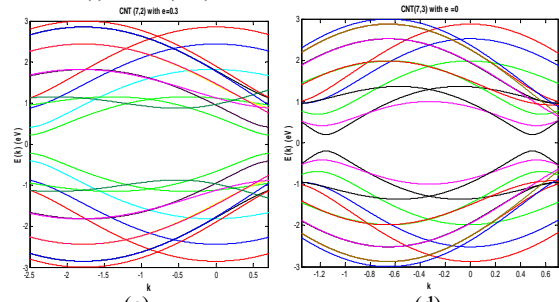

Fig.3. Relation of Energy Dispersion E(k) and k for
(a) CNT (7,2) e=0, (b) CNT (7,2) e=0.04, (c) CNT(7,2) e=0.4, (d) CNT (7,3) e=0, (e) CNT (7,3) e=0.04, (f) CNT (7,3) e=0.2, (g) CNT (8,0) e=0, (h) CNT (8,0) e=0.02, (i) CNT (8,0) e=0.05, (j) CNT (6,4) e=0, (k) CNT (6,4) e=0.04, (l) CNT (6,4) e = 0.2

It can be seen in Fig.1 and 2 that the energy gap shows two region which are noted as region 1 and region 2. The energy gap of (8,0), (7,2), (7,3) and (6,4) CNTs decrease with increasing the deformation parameter in region 1. The semiconductor-metal transition for (8,0) and (7,2) nano tubes can be seen at $e = 0.052$ with $E_g = 0.007$ eV and $e = 0.049$ with $E_g = 0.001$ eV, respectively. In region 1 the energy gaps decrease with increasing the deformation parameter. On the other hand in region 2, the energy gaps increase with increasing the deformation parameter. The diameter of both (8,0) and (7,2) tubes are 6.34 A^0 and 6.41A^0, respectively[10]. Even though the tube diameter 0f (7,2) is slightly larger than of (8,0), the band gap of (8,0) is near zero gap (metallic behavior) with the bigger deformation. Comparing Fig.3 (a), (b), (c),(e), (f) and (g), it shows that when $e = 0$ there is a gap related to the semiconductor properties. Moreover when $e = 0.04$, there is not a gap (metallic properties) and increasing on e at 0.4, there is a gap again (semiconductor properties). In Fig.2, (7,3) and (6,4) CNTs have the same deformation parameter when they show the metallic behavior that is 0.04 with $E_g = 0.005$ eV. It is very interesting to analysis this condition because their tube diameters are slightly different. The diameter of (7,3) and (6,4) CNTs are 6.96 A^0 and 6.83 A^0, respectively[10]. From Fig. 2, we can see that their energy gap back to the primary condition without deformation are at $e = 0.08$. If we see Fig.3 (d), (e), (f), (j), (k), and (l) and we compare them it seems that their shapes are slightly the same. There is a gap when the deformation parameter $e = 0$, following $e = 0.03$ there is no gap and $e = 0.2$ there is a another gap. Comparing with the result of Peng. S, et al, the deformation parameter is higher than of us. Using DFT method, they find $e = 0.25$ when (8,0) CNT shows the metallic behavior. It means that it needs a big pressure to make a metal-semiconductor transition.

These conditions of the metal-semiconductor transition can be further explored to utilize them for developing a switching device.

4. Conclusions

In conclusion, we have analyzed the metal-semiconductor transitions of (8,0), (7,3), (7,2) and (6,4) carbon nanotubes using tight binding method. We can change the electronic behavior of these CNTs with a small mechanical deformation. Our calculation about deformation effect on (8,0) CNT shows the same condition with the result of Peng.S, et al.

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