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Strain Effect on Transport Properties of Chiral Carbon Nanotube Nanodevice

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Abstract

The quantum transport properties of chiral single walled carbon nanotube (SWCNT) quantum dot nanodevice are investigated under the effect of tensile strain. This nanodevice is modeled as single walled carbon nanotube quantum dot connected to metallic leads. These two metallic leads operate as a source and a drain. The conducting substance is the gate electrode in this three-terminal nanodevice. Another metallic gate is used to govern the electrostatics and the switching of the carbon nanotube channel. The substances at the carbon nanotube quantum dot/ metal contact are controlled by the back gate. The electric current is deduced using Landauer-Buttiker formula. Results show that both energy gap and the electric current of the present nanodevice depend very sensitively on the chiral indices of SWCNT, its diameter and its chiral angles. Also, oscillatory behavior of the current is observed which is due to Coulomb blockade oscillations and Fano resonance. The present results are found to be in concordant with those in the literature, which confirm the correctness of the proposed model. This study is valuable for nanotechnology applications, e.g., soft and flexible nanoelectronics, nanoelectromechanical resonators and photodetectors.

Keywords

SWCNT Quantum Dot, Strain Effect, Ac-field, Magnetic Field, Nanodevice

1. Introduction

The advances in nanotechnology have brought new tools to the field of nanoelectronics and sensors [1]. New designed nanomaterials offer new and unique properties enabling the development and cost efficient production of state-of-the-art components that operate faster, has higher sensitivity, consume less power, and can be packed at much higher densities [2, 3]. Carbon atoms can form chemical bonds by hybridizing the atomic orbitals of their valence bonds and assume many structural forms such as graphite, diamond, carbon fibers, fullerenes, graphene and carbon nanotubes. Carbon nanotubes (CNTs) discovered by SumioIijima in 1991[4] , are one of the most exciting 1-D nanomaterials that exhibit fascinating electrical, optical, and mechanical properties such as high current density, large mechanical stiffness, and field emission characteristics [5, 6]. These properties of CNTs enable a wide range of applications in the various fields of nanoelectronics and sensors [5-9]. A single-walled carbon nanotube (SWCNT) is a graphene sheet rolled into a cylindrical shape with a diameter of about 0.7 - 2.0 nm [5, 10], but a multiwalled carbon nanotube (MWCNT) comprises a number of graphene sheets rolled concentrically with an inner diameter of about 5 nm [6, 7]. Carbon nanotubes (CNTs) according to their structures are classified to three types of armchair, zigzag, and chiral [10]. The terms 'zigzag' and 'armchair' refer to the arrangement of hexagons around the circumference. Armchair and zigzag nanotubes are defined by a carbon nanotube whose mirror image has an identical structure to the original one. On the contrary, chiral nanotubes in which the hexagons are arranged helically around the tube axis, exhibit a spiral symmetry whose mirror image cannot be superposed on to the original one [7, 10]. Also, carbon nanotubes (CNTs) are classified into the three groups according to values of chiral indices n and m [7, 10]:

Armchair carbon nanotubes - (n; n) C-C bonds are perpendicular to the tube axis.

Zigzag carbon nanotubes - (n; 0) C-C bonds are parallel to the tube axis.

Chiral carbon nanotubes - (n;m≠ n).

SWCNTs can be either metallic or semiconducting, depending on their diameter and chirality [7, 10]. One of the important things which plays essential role on electronic properties, is the energy gap which can inform us about metallic and semiconducting properties of nanotubes [11,12]. The strain has significant effects on the electronic properties of CNTs [13-16]. The authors [15] have shown that strain can change the conductance of a zigzag nanotube by several orders of magnitude. The pioneer experiment by Tombler et al. [17] shows that high strain (~3%) can change the conductance of a metallic single-walled nanotube by two orders of magnitude. In that experiment, strain was applied to a suspended nanotube using atomic force microscope (AFM) tip. Strain can open up a band gap in metallic CNTs, and can modify the band gap of semiconducting CNTs [11]. Small band gap semiconducting or quasi-metallic nanotubes exhibit the largest changes in resistance and piezo-resistive gauge factors, and they can be used as nanoscale pressure sensors [18, 19]. The present authors [20] studied the quantum characteristics of the single walled carbon nanotube (SWCNT) quantum dot under the effect of an external strain. Armchair SWCNT and Zigzag SWCNT with different diameters and chirality have been considered.

The purpose of the present paper is to investigate the quantum transport characteristics of single walled carbon nanotube quantum dot nanodevice under the influence of an ac-field (mid infrared region). The effect of tensile strain for chiral CNT will be taken into consideration.

2. The Model

The single walled carbon nanotube quantum dot nanodevice can be modeled as follows: A single walled carbon nanotube in the form of quantum dot is connected to two metallic leads. These two metallic leads operate as a source and a drain. The conducting substance is the gate electrode in this three-terminal nanodevice. Another metallic gate is used to govern the electrostatics and the switching of the carbon nanotube channel. The substances at the carbon nanotube quantum dot / metal contact are controlled by the back gate. The Dirac fermion electron tunneling through the present investigated nanodevice is induced by an external applied ac-field which is expressed as:

$$V = V_{ac}\cos\omega t \tag{1}$$

where Vac is the amplitude of the ac-field and ω is its frequency. Using Landauer-Buttiker formula, the electric current, I, is given by [20-23].

$$I = \frac{4e}{h}\int_{E_F}^{E_F+n\hbar\omega} dE.[f_{FD(s)}(E) - f_{FD(d)}(E - eV_{sd})]\Gamma_{withPhoton}(E) \tag{2}$$

where $\Gamma_{withphotons}(E)$ is the photon-assisted tunneling probability, $f_{FD(s)}$ & $f_{FD(d)}$ Fermi-Dirac distribution functions corresponding to source and drainleads respectively ,V_{sd} is the bias voltage, E is the energy of tunneled electrons and e is the electronic charge and h is the Planck's constant. The photon assisted tunneling probability, $\Gamma_{withPhoton}(E)$ could be expressed in terms of the tunneling probability without photons $\Gamma_{withoutPhotons}(E - n'\hbar\omega)$, as follows [21-25]:

$$\begin{aligned}\Gamma_{withPhoton} = \sum_{n'=1}^{\infty} J_{n'}^{2}\left(\frac{eV_{ac}}{n\hbar\omega}\right)\times \\ f_{FD}\left(E - \left(\frac{C_{CNT}}{C}\right)eV_g - n'\hbar\omega - eV_{sd}\right)\times \\ \Gamma_{withoutPhotons}(E - n'\hbar\omega)\end{aligned} \tag{3}$$

where C_{CNT} is the capacitance of the SWCNT quantum dot, C is the coupling capacitance between CNT quantum dot and the leads, Vg is the gate voltage, $\hbar\omega$ is the energy of the induced photon and $J_{n'}$ is the n'^{th} order Bessel function corresponding to the n'^{th} different side bands of nanostructure carbon nanotube. The tunneling probability without the induction of the photons $\Gamma_{withoutPhotons}(E - n'\hbar\omega)$ could be determined using the WKB approximation method [26, 27] as follows:

$$\begin{aligned}\Gamma_{withoutphoton}(E - n'\hbar\omega) = \\ \exp\left[-2\int_{d}^{d+\Delta} dx \times \left(E_g/\sqrt{3}a\gamma_o\right)\times \right. \\ \left. \sqrt{1 - \left(\left(\begin{matrix}E_1 - n'\hbar\omega + \\ eV_{sd}(1 - x/L)\end{matrix}\right)\Big/\left(E_g/2\right)\right)^2}\,\right]\end{aligned} \tag{4}$$

where a is the lattice constant, γ_o is the nearest neighbor hopping integral, Eg is the strained band gap energy, L is the length of SWCNT quantum dot, d is the diameter of SWCNT and Δ is its thickness. The energy, E1, (Eq.4) is given by:

$$\begin{aligned}E_1 = E_F + eV_g + V_b + \frac{N^2e^2}{2C_{CNT}} + \\ eV_{ac}\cos(\omega t) + \frac{\hbar eB}{2m^*}\end{aligned} \tag{5}$$

where E_F is the Fermi-energy, V_b is the barrier height at the interface between SWCNT quantum dot and leads, N is the number of tunneled electrons and e is the electronic charge, B is the applied magnetic field and m* is the effective mass of the charge carrier. The strained band gap energy, E_g, of chiral single walled carbon nanotube is expressed in terms of the induced tensile strain, ε, as follows [13]:

$$E_g = \left| \left(\frac{\pi^2 \gamma_0}{8 C_h^5} + \frac{a b \sqrt{3}}{4 C_h^3} . \varepsilon \right) (n-m)\left(2n^2 + 5nm + m^2\right) \right| \tag{6}$$

where b is the linear change in the transfer integral with a change in bond length due to strain and C_h is the chiral vector with chiral indices n and m. This chiral vector, C_h, is expressed as [10, 28]:

$$C_h = \sqrt{n^2 + nm + m^2} \tag{7}$$

The diameter, d, of SWCNT and the chiral angle, θ, are determined in terms of the chiral indices n and m [10, 28] using the following equations :

$$d = \frac{a}{\pi}(n^2 + nm + m^2)^{\frac{1}{2}} \tag{8}$$

and

$$\cos\theta = \frac{2n+m}{2\sqrt{n^2 + nm + m^2}} a \tag{9}$$

In the present paper we consider only chiral single walled carbon nanotube with chiral indices n, and m [7, 10].

3. Results and Discussion

Numerical calculations are performed for the strained energy gap energy, Eg, for chiral SWCNT (Eq.6). The values of parameters are: the lattice constant a= 2.46Å & the nearest neighbor hopping integral γ_0= 2.6 eV [30]. The value of the parameter b= 3.5 eV/Å [13, 29]. The table 1 below shows the values of diameter, d, and chiral angle,θ, for the chiral SWCNT:

Table 1. *The values of diameter and chiralangle of Chiral SWCNT with different chiralindices.*

(6,2)	(6,3)	(8,3)
5.649Å	6.218Å	7.716Å
14.060	19.090	15.200

It is well known that for chiral SWCNT with chiral indices n & m shows the metallic characteristics when (2n+m)/3 is an integer, otherwise they are semiconducting [7, 10]. In the present paper we see that chiral (6, 3) is metallic, while the others chiral (6,2) and chiral (8,3) are semiconductors.

- Figure 1 shows the variation of energy gap, Eg, for chiral SWCNTs of different chiral indices (Figure 1) with strain. The energy gap, Eg, varies linearly with strain. It is noted from this figure for metallic chiral SWCNT with chiral indices (6,3) that its energy gap is modulated with strain very small (Figure 1 blue line) which shows a metallic SWCNT to semiconducting SWCNT transition [20,29,31]. While for semiconducting SWCNT (see Figure 1, red and black lines) the energy gap decreases as the chiral indices, n and m increases at the same value of strain. This is expected result for chiral semiconducting SWCNT according to Eq.6. From this figure we see that the variation of the energy gap, for the present studied chiral SWCNT, with strain is very sensitive to the chiral indices and the corresponding diameter and the chiral angles. The present results are found concordant with those in literature [7, 13, 20, 21, 29]. The variation of energy gap of chiral metallic and semiconducting SWCNT with strain might be due tobreaking the bond symmetry due to curvature of nanotube [10, 20, 21, 31].

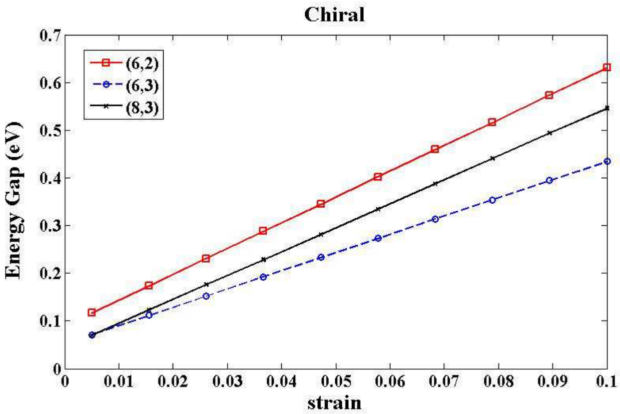


Fig. 1. *The variation of energy gap with strain for chiral SWCNT with different chiral indices.*

It is interesting to investigate the variation of the electric current (Eq.2) with strain for the present studied SWCNT quantum dot nanodevice under the influence of an ac-field in the mid-infrared region and magnetic field. So, numerical calculations are performed for the current, I, (Eq.2) for chiral SWCNT. The values of parameters for SWCNT quantum dot: C= 0.4 nF, CCNT= 0.25 nF, eVac= 1 meV, L=20 nm and Vb= 0.3 eV [21, 23, 24]. The values of the source-drain voltage and temperature are 0.2 V and 150K respectively. The optimum value of Fermi energy, E_F, was taken as, approximately, equals 1 eV [32, 33]. Effective mass of the charge carriers is an important parameter for the electrical transport properties of SWCNTs and its variation with the energy gap, Eg, at energies approaching the band minimum [7] is given by:

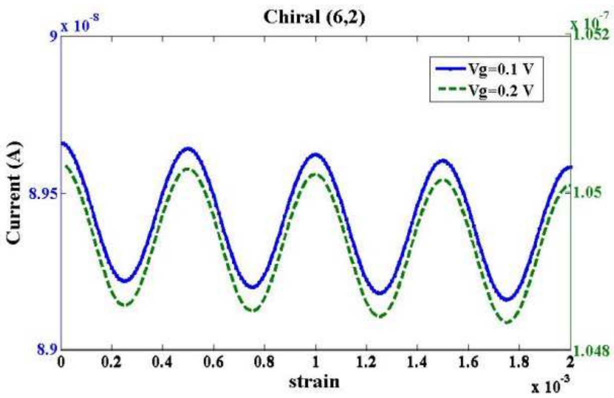
$$m^* = \frac{4\hbar^2}{3\gamma_0 a^2} . \frac{E_g}{2\gamma_0 + E_g} \tag{10}$$

Now computing the effective mass, m*, corresponding to the strained energy gap (Eq.10) and we take the most optimum value which is m*= 0.054 me [21, 23, 24].

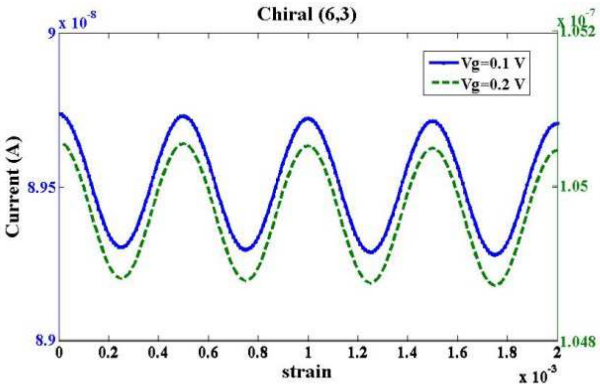
The features of the present results are the following:

-Figure 2 shows the variation of the current with the tensile strain for the present investigated chiral SWCNT quantum dot nanodevice at different values of the gate voltage. As shown from this figure that periodic oscillations of the current with nearly equal peak separation. This oscillatory behavior of the current is due to the Coulomb blockade oscillations [20, 23, 24]. According to the present investigated nanodevice, the top gate allows the coupling strength between the leads and the ballistic channel to be controlled. Because of the confinement, both transverse and longitudinal motion of the charge carriers in 1D channel are quantized, giving rise to a set of distinct energy levels. The present results are found to be concordant with those in the literature [34-36].

-Figure 3 shows the variation of the current with strain at different values of the frequency of the induced ac-field in the mid-infrared region. The oscillatory behavior of the current with strain might be explained as follows: The effect of ac-field on the transport through the nanodevice might be achieved for those charge carriers with energy component, E, E±ħω, E±2ħω, ………, where ħω is the photon energy of the ac-field [23-25]. These energy components are called side bands [34-36]. A positive value is due to the absorption of n-photons (n=1, 2, 3, …..) and anegative value is due to the emission of photons during the tunnel process. The observed peak height is determined by Bessel function (see Eq.3) [25, 36]. Also, we notice that the peak height increases as the photon energy increases. This enhancement of the current might be due to the photon induced side-bands resonances [23-25, 36, 37]. The interplay between the transport of charge carriers and the induced photons increases strongly as the energy of theses photons increases. As a consequence of this interplay, that is, this interplay affects on the side-bands and the tunneling rates [23-25, 36, 37].



(a)



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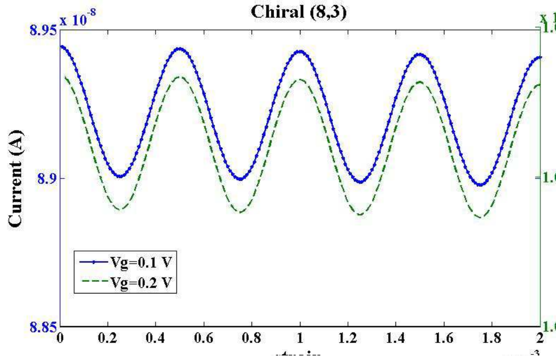
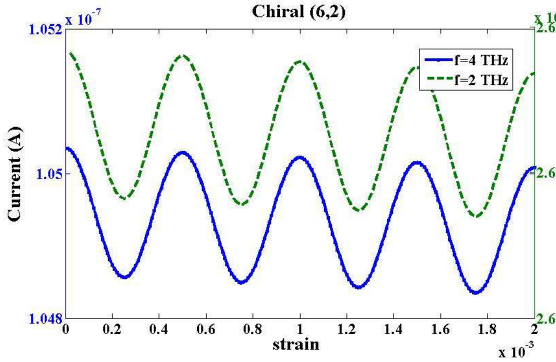
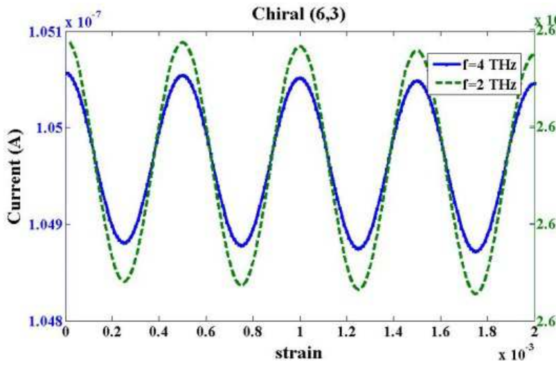


(c)

Fig. 2. *The variation of the current with strain for the studied chiral SWCNTs at different values of gate voltage.*



(a)



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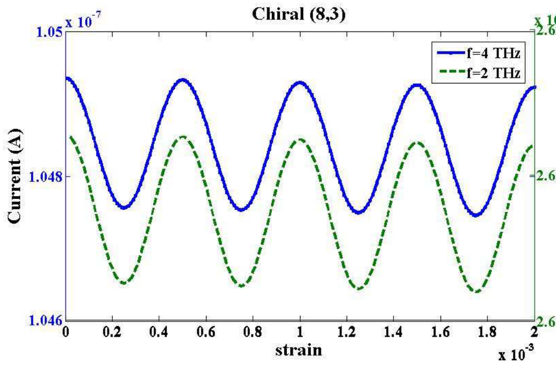
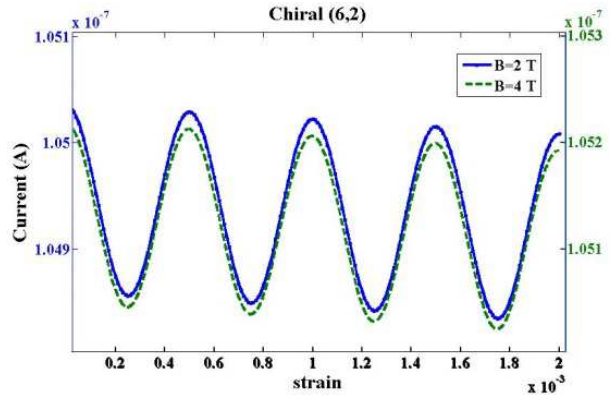


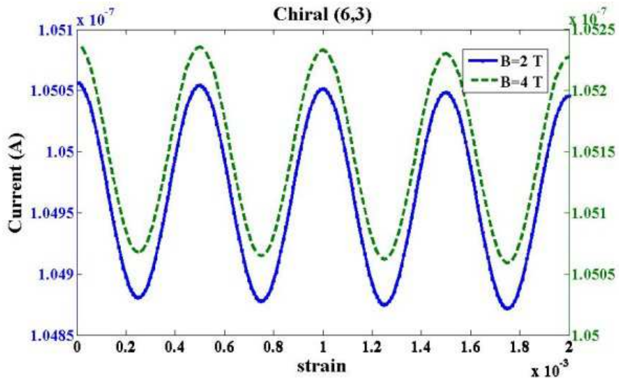
(c)

Fig. 3. *The variation of the current with strain at different values of the frequency of the induced ac-field.*

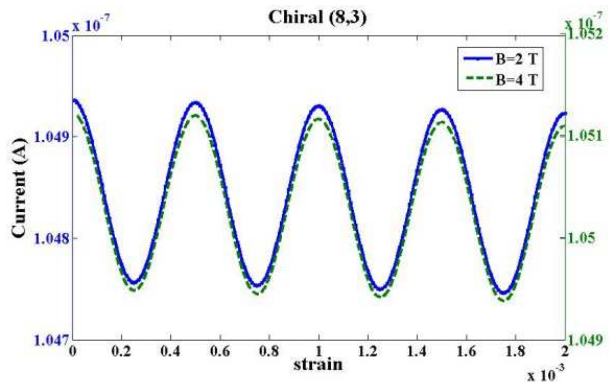
-Figure 4 shows the variation of the current with strain at different values of the applied magnetic field. A periodic oscillation of the current is observed and it is noticed from this figure that the effect of magnetic field on the transport of charge carriers depends on the chiral indices n, m and correspondingly on the diameter of SWCNT and the chiral angle. It is known that the influence of an external magnetic field will lead to a change in the energy level separation between the ground state and the first excited state in SWCNT quantum dot [23, 37, 38]. Also, the magnetic field affect on the photon-assisted tunneling rates between electronic states of the SWCNT quantum dot.



(a)



(b)



(c)

Fig. 4. *The variation of the current with strain atdifferent values of the applied magnetic field.*

As shown from Figures 2, 3, 4, a periodic oscillation of the current with the strain. These oscillations are Coulomb blockade oscillation [23, 24]. Also, according to the present model of single walled carbon nanotube quantum dot nanodevice, the interaction of the tunneled electrons with the induced ac-field leads to photon-mediated transmission resonances. The interplay between the induced photons and the tunneled electrons leads to what it is known as Fano-resonance [39].In general, the oscillatory behavior of the current might be due to Fano-resonance as the quantum transport of electrons is performed from continuum states of leads to the discrete states of nanostructure SWCNT quantum dot [39]. The observed periodic oscillation of the current with strain for chiral SWCNT quantum dot nanodevice might be operated as single electron transistor [34]. Results of the present paper show that SWCNT quantum dot nanodevice might be applied in the field of soft and flexible nanoelectronics [40].

4. Conclusion

We conclude from the present investigation that the present nanodevice could be used as a photo-nanoscopic device for frequencies in the THz region. Also, the SWCNT quantum dot could find applications in microwave communications, imaging systems and nanoelectromechanical devices for strain sensing in nanostructure materials.

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