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Band Structure Variation for SWCNTs under Deformation

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Abstract

The electronic properties of single walled carbon nanotubes (SWCNTs) influenced by the mechanical elastic deformation are investigated by using a tight-binding approximation. We analyze the band structure for SWCNTs in a wide range of energies around a Fermi energy level. Our work includes the uniaxial, torsional and sub-lattice deformation, which is applied to modify the electronic transport properties of SWCNTs, e.g. the energy spectrum as a function of the deformation tensor. However, the results showed that the electronic properties of SWCNTs are affected by deformation processes, where the energy spectrum is changed perceptibly.

Keywords: SWCNTs; Tight-binding Approximation; Energy spectrum; Energy Gap; Elastic deformation.

1. Introduction

A carbon nanotube has a quasi-one dimensional structure. Geometrically, a carbon nanotube can be represented as a seamless cylinder which is achieved by rolling up a section of a graphene sheet, followed by gluing its opposite sides [1]. Wallace showed that the band structure of graphene has no energy gap and that the energy spectrum of electrons and holes at the points of contact between the valence and conduction bands is linear [2]. The transformation of an electronic spectrum during the elastic deformation of structures that have translational symmetry was analyzed in Ref. [3].

The specific mechanical and electronic properties of single walled carbon nanotubes (SWCNTs) make it a good candidate material for use in many nanoelectromechanical systems (NEMS) [4–6]. The electronic properties are found to be extremely sensitive to uniaxial and torsional deformation [7,8], that allow to predict the development of the nanodevices and nanoelectronics based on SWCNTs. Various methods have been proposed or implemented to tune the electronic properties of SWCNTs. Tomblor et. al. confirmed the dependence of the electrical conductivity on the bending of SWCNTs by the tip of AFM [9]. It was

found that the electrical conductivity changed twice as a result of the elastic mechanical deformation.

Earlier studies of the energy gap modification for zigzag and armchair SWCNTs that depend on the mechanical strain have shown interesting behaviors [10–12]. The effect of the uniaxial strain was studied by using a Green's function method based on the π electron approximation and four orbital numerical methods in Ref. [10] and Ref. [11] respectively. Ref. [12] predicted the opening of the energy band gap in armchair SWCNTs under a torsional deformation, using a method that wraps a massless two dimensional Dirac Hamiltonian on a curved surface. Theoretical calculations were achieved for the energy spectrum of π -electrons in SWCNTs depending on the magnitude of the elastic deformation, represented by a uniaxial (tension – compression) and a torsional deformation [13]. A simple and accurate method to determine the atom positions in uniformly deformed SWCNTs were developed by B. Liu et.al [14] via a continuum analysis based on the interatomic potential. Seon-Myeong Choi et. al. presented a new scheme to induce shear strain in one-dimensional materials like SWCNTs without introducing artificial edge atoms[15].

The mechanical deformation represented by the nanoplasticity of SWCNTs under uniaxial compression is investigated using generalized tight-binding molecular dynamics, and *ab initio* electronic structure methods devised by D. Srivastava et. al.[16], they found that at the elastic limit (for 12% compression of zigzag CNT (8,0)), the relaxation of the compressed CNT resulted in a spontaneous plastic collapse. Consequently, the interplay between mechanical and electronic properties may be useful in

many applications of nano-devices based on SWCNTs [17].

In the present work, the electronic density of states (DOS) and the band structure characteristics of SWCNTs have been studied under the influence of three patterns of mechanical deformation: uniaxial, torsional and sub-lattice deformation represented by the reconstruction of the sub-lattice or relative displacement of atoms. Three orientations of SWCNTs have been taken under consideration in our study: zig-zag(10,0), armchair(5,5) and chiral(8,2).

2. Computational Details

The structure of a SWCNT can be characterized by a chiral vector $\vec{C} = i_1 a_1 + i_2 a_2$, where a_2 and a_1 are the basis vectors of graphene lattice, i_2 and i_1 are the chiral indices. Armchair and zigzag carbon nanotubes correspond to the chiral angle $\theta = 30$ and 0 , respectively, as shown in Fig. 1. The periodicity condition of the electron wave function in the transverse direction of the graphene strip, leads to the quantization of the transverse components of the wave vector, and an energy gap be appear in the band structure of CNTs due to the quantization process. The procedure of rolling graphene sheet leads to the identification of the points on the opposite sides of the strip that are spaced by vector \vec{C} , and the edges of the strip are represented by the parallel lines that pass through the ends of vector \vec{C} . A cylindrical surface built up as a result of rolling the strip is considered, so that the basis translational vectors a_1 and a_2 are transformed into helical twists operators $S_1(\Delta\phi_1, \Delta z_1)$ and $S_2(\Delta\phi_2, \Delta z_2)$ on the cylindrical surface of radius $R = |\vec{C}| / 2\pi$, where $(\Delta\phi_1, \Delta z_1)$ and $(\Delta\phi_2, \Delta z_2)$ - the

parameters of helical twists operators, can be determined geometrically as follows (see Fig. 1),

$$\begin{aligned}\Delta\varphi_1 &= \sqrt{3} a_0 \cos \theta / R, \\ \Delta\varphi_2 &= \sqrt{3} a_0 \cos(\frac{\pi}{3} - \theta) / R, \\ \Delta z_1 &= -\sqrt{3} a_0 \sin \theta, \\ \Delta z_2 &= \sqrt{3} a_0 \sin(\frac{\pi}{3} - \theta)\end{aligned}\quad (1)$$

where a_0 is the distance between the nearest neighbor atoms in undeformed sheet of graphene.

The rules of the helical twists operators are determined as follows: the helical twists operators $S_1(\Delta\varphi_1, \Delta z_1)$ on the point of the cylindrical coordinate (φ, z, R) lead to the arbitrary coordinates points $(\varphi, z, R) \rightarrow (\varphi + \Delta\varphi, z + \Delta z, R + \Delta R)$. The atomic structure of CNTs results from measuring the helical twists operators $S_1^j(\Delta\varphi_1, \Delta z_1) S_2^n(\Delta\varphi_2, \Delta z_2)$ per unit cell of a CNT, where j and n are any integers per unit cell of CNT. For the values of j and n that are equal to the chiral indices of the CNT, we have:

$$S_1^{i_1}(\Delta\varphi_1, \Delta z_1) S_2^{i_2}(\Delta\varphi_2, \Delta z_2) = I \quad (2)$$

Consequently, the parameters of the helical twists operators (2) satisfy the following condition [13]:

$$i_1 \Delta\varphi_1 + i_2 \Delta\varphi_2 = 2\pi, \quad i_1 \Delta z_1 + i_2 \Delta z_2 = 0 \quad (3)$$

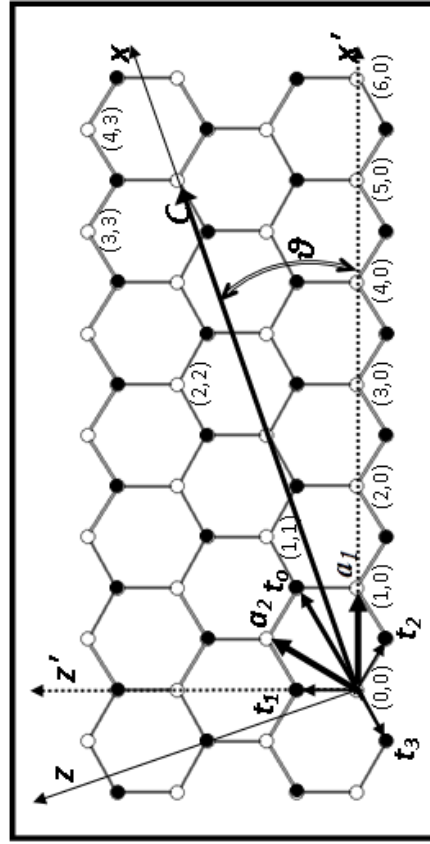


Fig.1: Atomic Structure and the basis vectors for the construction of SWCNT [13].

The tight binding approximation is used to describe the matrix elements of the Hamiltonian operator of carbon nanotubes that determine the amplitudes of electron transitions between the nearest neighbor's atoms, which are calculated through the wave functions of the π -electrons. For carbon systems, the researchers use the parametric exponential functions to determine the dependences of the matrix elements on the interatomic distance, where r_{12} is the vector connecting the atoms with conventional numbers 1 and 2. We use the parametric functions for the matrix elements of the Hamiltonian operator of π electrons as follows [18],

$$\beta(|r_{1,2}|) = \beta \exp(-3.37(|r_{1,2}|/a_0 - 1)) \quad (4)$$

where the energy parameter is $\beta = 2.7$ eV.

In the tight binding approximation, the electron energy is determined through two quantum numbers, namely, magnetic quantum number $m = 0, \pm 1, \pm 2, \pm 3, \dots$ and wave vector k , as follows:

$$E_{m,k}^{\pm} = E^0 \pm |H_{m,k}^{A,B}| \quad (5)$$

$$H_{m,k}^{A,B} = \beta_1 e^{-i(m\Delta\phi_1 + k\Delta z_1)} + \beta_2 e^{-i(m\Delta\phi_2 + k\Delta z_2)} + \beta_3 e^{-im(\Delta\phi_1 + \Delta\phi_2) - ik(\Delta z_1 + \Delta z_2)}$$

where $\beta_{1,2,3}$ represents the matrix elements built on atomic wave functions which determine the amplitudes of the electron transition among the nearest atomic neighbors on a carbon nanotube. The signs \pm in formula (3) refer to the two energy bands, E_0 is the energy of binding π -electron with a free carbon atom, its value equal to zero.

The uniform deformation of a carbon nanotube can be seen as a result of the continuous transformation of the coordinates of the points located on the nanotube surface, $(\phi, z, R) \rightarrow (\phi', z', R')$, where (ϕ', z', R') are the point coordinates after deformation. Here, we have [13]:

$$\phi' = \phi + z \times \gamma_1 / R, \quad z' = z \times (1 + \gamma_2) \quad (6)$$

$$R' = R \times (1 + \gamma_3)$$

where $\gamma_1, \gamma_2, \gamma_3$ are the dimensionless deformation parameters. The elastic uniaxial deformation of a nanotube is described by a set of parameters $\gamma_1 = 0, \gamma_3 = -\nu \times \gamma_2$, where ν is the Poisson ratio, the dimensionless parameter γ_2 determines the magnitude of the uniaxial deformation. This ratio is assumed to be independent of the chiral angle θ and equal to the Poisson ratio of graphene ($\nu = 0.17$).

The torsional deformation can be represented as the relative rotation of the cross section of CNT; correspondingly, we choose parameters $\gamma_2 = 0, \gamma_3 = 0, \gamma_1$ to

determine the angle of rotation. According to Eq. (4), the elastic deformation changes the parameters of helical twist operators $(\Delta\phi_1, \Delta z_1)$ and $(\Delta\phi_2, \Delta z_2)$ as follows [13]

$$\Delta\phi'_{1,2} = \Delta\phi_{1,2} + \Delta z_{1,2} \times \gamma_1 / R, \quad (7)$$

$$\Delta z'_{1,2} = \Delta z_{1,2} \times (1 + \gamma_2),$$

Formula (7) allows us to determine the cylindrical coordinates of the sub-lattice A atoms in the deformed CNT.

From eq. (7), we can determine the cylindrical coordinates of the sub-lattice A atoms in CNT after deformation. One can find the cylindrical coordinates of sub-lattice B atoms by applying eq. (6) in the formula of the helical twist operators, which allow us to calculate the cylindrical coordinates of the sub-lattice B atoms belonging to the isolated (zero) unit cell. And then by using the helical twists operators $S_1(\Delta\phi_1, \Delta z_1)$ and $S_2(\Delta\phi_2, \Delta z_2)$, one can define cylindrical coordinates of other atoms of the sub-lattice B.

We now consider another type of the atomic deformation, namely, the restructuring of a carbon nanotube associated with a relative geometrical displacement of the two sub-lattices A and B individually. In the case of graphene, the displacement of sub-lattices A and B can be performed perpendicularly or tangentially to the plane. Correspondingly, restructuring CNT can be achieved via the displacement of sub-lattices A or B by the rotational or the longitudinal shift according to the following rule [13]:

$$(\phi_A, z_A, R) \rightarrow (\phi_A, z_A, R), \quad (8)$$

$$(\phi_B, z_B, R) \rightarrow (\phi_B + \delta\phi, z_B + \delta z, R + \delta R)$$

Here, $(\phi_A, z_A, R), (\phi_B, z_B, R)$ are the cylindrical coordinates of the atoms of sub-lattices A and B, respectively; $\delta\phi$ is the relative rotation of the sub-lattices B, and δz is the shift of sub-lattice B along the CNT axis.

3. Results and discussion

3.1. Atomic Structure of CNTs under Deformation

The atomic structure of deformed CNTs is illustrated in Fig. 2. Panels a , b and c show CNTs of zig-zag orientation(10,0) under a relative sub-lattice deformation in the uniaxial (a), torsional (b) and radial directions (c) respectively. From schematic figures of the deformed CNTs (see Fig. 2), the new reconstructed structure arises due to the geometrical modification in the operators \hat{S}_1 and \hat{S}_2 affected by three patterns of the deformation under consideration. Furthermore, the bond length between the nearest atoms or the length of the connecting vectors t_0 , t_1 , t_2 and t_3 are changed differently depending upon the orientation of CNTs and the way of deformation.

Thus, the magnitude of the parametric function of the matrix elements β_0 , β_1 and β_2 will change according to the length of the connecting vectors t_0 , t_1 , t_2 and t_3 respectively.

3.2. Energy Spectrum of Deformed CNTs

One of the characteristic manifestations of the mechanical deformation in CNTs is the change of the energy spectrum or the electronic dispersion behavior under the influence of deformation as shown in Fig. 3.

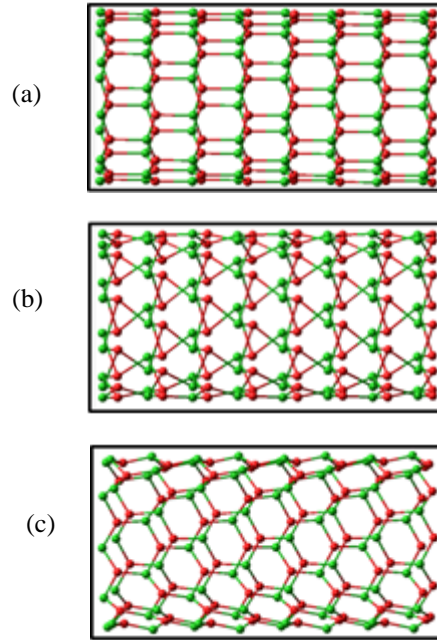


Fig.2. Samples of CNT (10,0) under relative sub-lattice deformation in an uniaxial direction(a), torsional direction (b) and radial direction (c).

We have adopted the energy dispersion relation represented by formula (5), which depends mainly on the magnetic quantum number m and wave number k , it has been used to investigate the influence of the elastic mechanical deformation on the energy spectrum of the valence and the conducting bands of zig-zag, armchair and chiral CNTs.

Fig.3 (a) shows the one-dimensional energy spectrum for undeformed zig-zag CNT (10,0), where the deformation parameters are zero ($\gamma_1 = 0, \gamma_2 = 0$), the sub-bands of the energy spectrum are observed. The energy spectrum includes each of valence and conduction bands (lower and upper band respectively) for each magnetic quantum number m .

Each one corresponds to a magnetic quantum number m resulting from the quantization of the wave vector k_x along the carbon nanotube circumference.

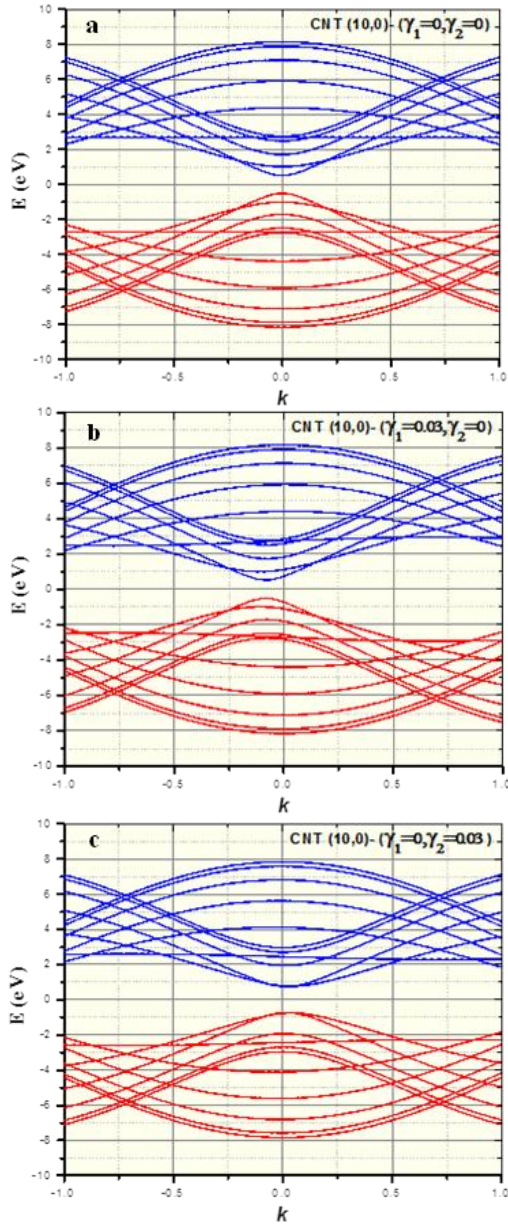


Fig.3. Energy Spectrum of CNT (10,0) under elastic deformation: undeformed CNT(a), uniaxial deformation (b) and torsional deformation (c).

According to the well-known relationship that determines the type of CNTs as a conductor or semiconductor, the undeformed zig-zag CNT(10,0) is represented as a semiconductor CNT with an energy gap of order approximately ≈ 1 eV as shown in Fig.3(a). Fig. 3(b) shows the effect of the torsional deformation on the energy spectrum. There is a slight change in the energy bands behavior at the

value of the torsional parameter $\gamma_1=0.03$. Our results coincide with those in Ref.[14], where they investigated the energy gap variation under the effect of a torsional strain. The variance in the energy spectrum pattern is apparent in one of the sub-bands which corresponds to the magnetic quantum number $m = 3$.

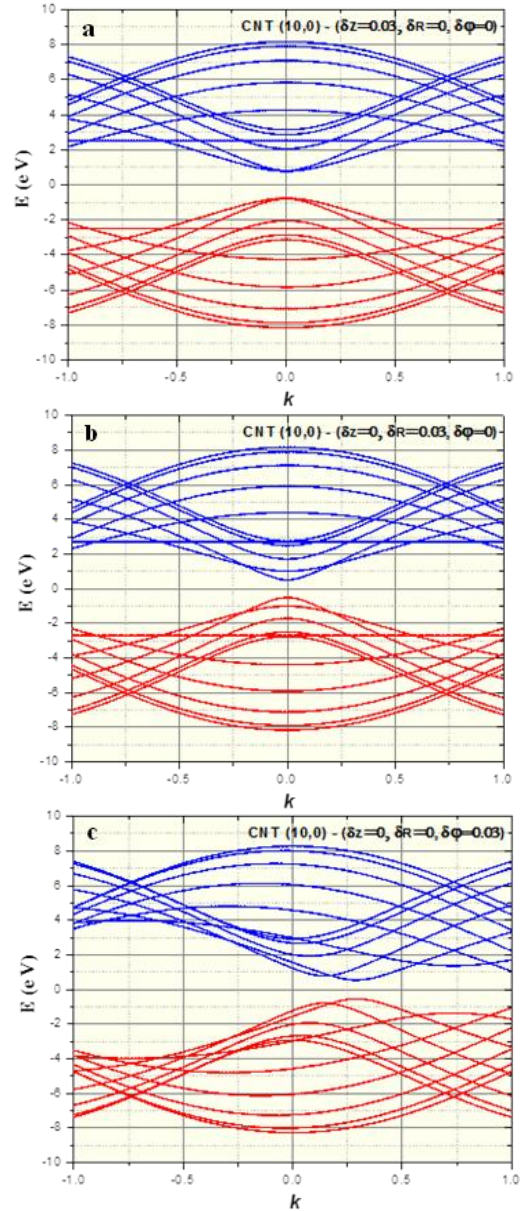


Fig.4. Energy Spectrum of CNT (10,0) under a relative sub-lattice deformation in an uniaxial direction(a), radial direction (b) and torsional direction (c).

The uniaxial deformation effect (the tension applied along the CNT axis) appears in Fig. 3(c), where the energy gap increases by 0.3eV, which is consistent with the results of Ref. [14].

Fig. 4 (a, b, c) shows the effect of the sub-lattice deformation on the energy spectrum of zig-zag CNT (10,0). The displacement parameters are included in our calculations $\delta_z, \delta_\phi, \delta_R$ which correspond to the sub-lattice *B* in the longitudinal, angular/transversal and radial directions respectively, where the displacement ranging between (0.1-0.3). It's evident by comparing Fig. 3(c) and Fig. 4(a), that they match in their behavior of the energy spectrum for the same values of the deformation and displacement parameters $\gamma_2 = \delta_z = 0.03$. This implies that the uniaxial and sub-lattice deformation in the longitudinal direction have the same effect on the energy gap opening. It is interesting as it appear clearly in Fig. 4(b), that sub-lattice deformation along the radial direction has no significant effect on the energy spectrum and consequently the electronic properties remain unchanged under deformation. By applying the sub-lattice deformation along the angular/transversal direction, the arrangement of the energy sub-bands lines in the energy spectrum are changed randomly, while the energy gap remains the same, ranging the maximum valence and minimum conduction bands as shown in Fig. 4 (c). The current study included a second type of CNTs, which corresponds to chiral angle $\theta = 30$ represented by the armchair with chiral indices (5,5). These CNTs are characterized by being conducting materials (i.e. with a zero energy gap) as shown in Fig. 5 (a). Fig.5 (b) illustrates the process of opening the energy gap in order of 0.4 eV due to the torsional deformation up to $\gamma_1 = 0.03$. On the

other hand, the armchair CNTs are not affected by the process of the uniaxial deformation in the longitudinal direction along the axis of CNT, as illustrated in Fig. 5 (c).

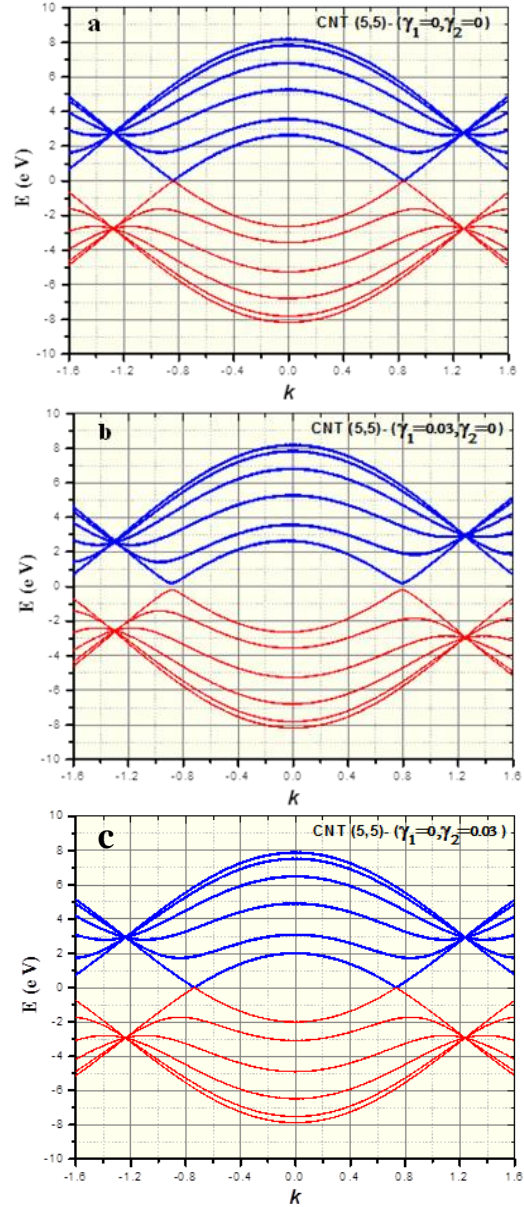


Fig.5. Energy Spectrum of CNT (5,5) under deformation: undeformed CNT, (a)uniaxial deformation, (b) and torsional deformation (c).

The energy spectrum of armchair CNTs can be tuned by applying the longitudinal and radial sub-lattice deformation. Thus, a small energy gap up

to 0.3 eV arises as a result of deformation in order of 0.03, as shown in Figs. 6 (a) and (c) respectively. In contrast, the angular/transversal sub-lattice deformation does not change the essential properties of the armchair CNTs.

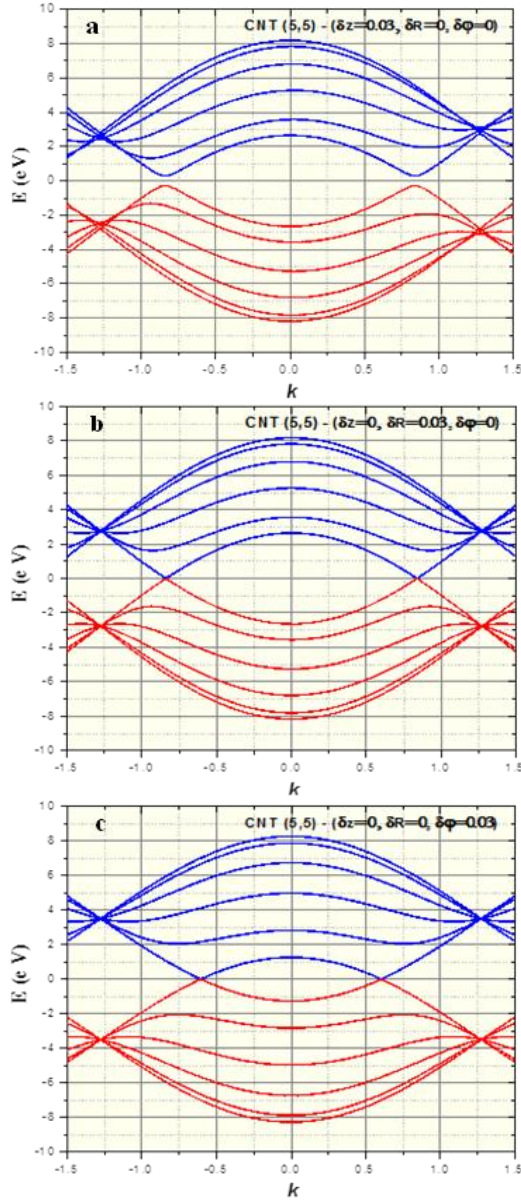
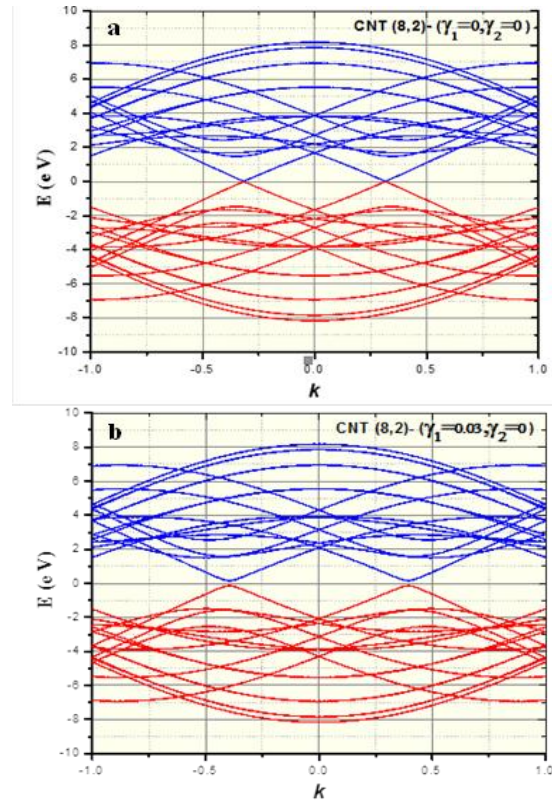


Fig.6. Energy Spectrum of CNT (5,5) under a relative sub-lattice deformation in the uniaxial direction(a), radial direction (b) and torsional direction (c).

where the chirality angle is $0 < \theta < 30$, and is characterized by the conducting CNTs according to the following rule: $i_1 - i_2 = 3n$, where n is integer. Fig. 7 (a) shows conducting CNT at the absence of the energy gap between the highest and lowest values of valence as well as the conducting bands in the energy spectrum respectively. By applying a torsional deformation of order $\gamma_1 = 0.03$, the energy gap will open in the limit of $\approx 0.2\text{eV}$, thus, the electronic properties change from conducting to semi-conducting as illustrated in Fig. 7(b). Fig. 7(c) shows the energy spectrum resulting from applying the uniaxial deformation of the same value of deformation parameter $\gamma_2 = 0.03$, its make clear that the energy gap opens up slightly more than the torsional deformation.



The chiral CNTs with the chirality indices (8,2) have been taken into account,

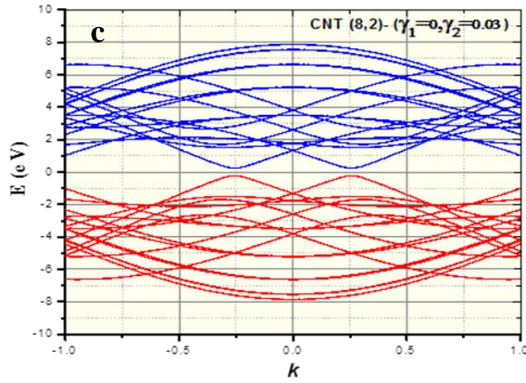


Fig.7. Energy Spectrum of CNT (8,2) under elastic deformation: undeformed CNT(a), uniaxial deformation (b) and torsional deformation (c).

Finally, the metallic electronic properties can be modified to become semi-conducting under the influence of a

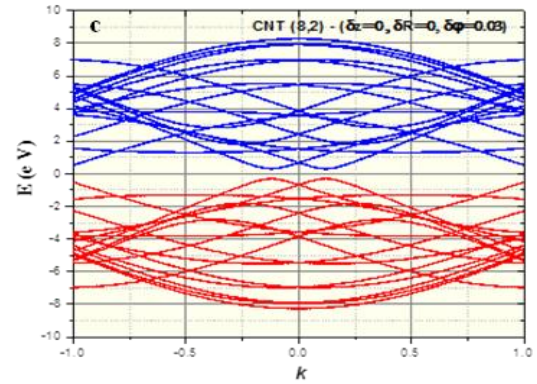
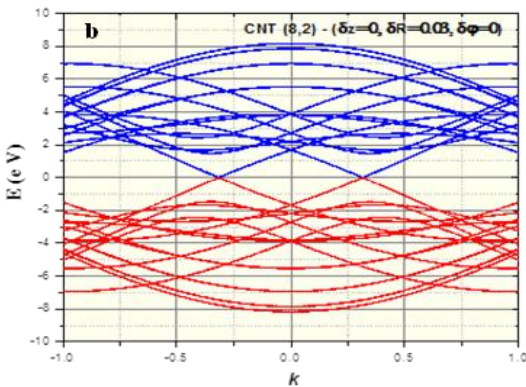
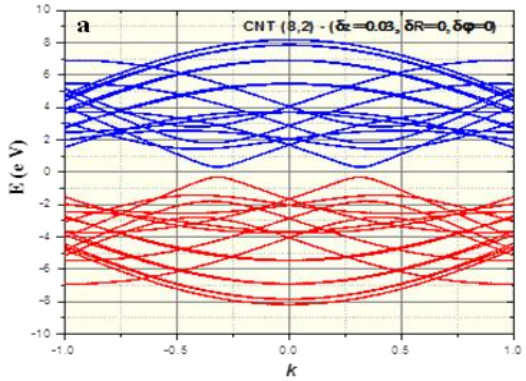


Fig.8. Energy Spectrum of CNT (8,2) under relative sub-lattice deformation in uniaxial direction(a), radial direction (b) and torsional direction (c).

sub-lattice deformation in the longitudinal and angular directions as illustrated in Figs.8 (a) and (c) respectively. In contrast, the CNTs remain metallic under a sub-lattice deformation in the radial directions, as shown in Fig. 8(b).



4. Conclusions

In summary, we have proved in our study that a tight-binding approximation is appropriate to predict very interesting properties of CNTs by applying three patterns of the elastic deformation. Consequently, the energy gap in the energy spectrum or the electronic properties of the low dimensional systems such as CNTs can be modified by controlling the displacement between the nearest neighbor atoms in the real space. Our numerical calculations demonstrate that all the patterns of deformation: including the unconventional pattern of sub-lattice deformation can yield new structures of the modified CNTs, which leads to a different dispersion relation. Thus, by using the tight-binding approximation with the parametric matrix elements of the Hamiltonian operator, which depends on the distance between the nearest atoms, it is shown that CNTs can be transformed

from conducting to semiconducting materials and vice versa. This may correspond to different materials or a new allotrope of carbon nanostructure which is characterized by novel electronic properties. The calculations presented in our study are motivated by the recent experimental progress in the field of nano-electronics and nano-devices based on CNTs. Obviously, in our theoretical calculations, the energy spectrum entirely depends on the chiral indices (i_1 , i_2) and the radius of CNTs.

We conclude that the electronic properties of zig-zag CNTs represented by the energy spectrum do not change clearly when the CNTs are exposed to the torsional mechanical deformation for any value of the deformation parameters within reasonable limits of (approximately) γ_1 and $\gamma_2 \leq 0.03$. These properties may be affected when the CNTs are subjected to the tension process such as the uniaxial deformation and the sub-lattice or relative displacement in the longitudinal and angular directions, but along the line, these properties are not at all affected by the sub-lattice deformation in the radial direction.

The electronic properties of armchair CNTs are affected by the uniaxial, torsional and sub-lattice deformation in both the longitudinal and angular directions, and are not affected by the sub-lattice deformation in the radial direction. Finally, the chiral CNTs are affected by all the patterns of deformation which are considered in our treatment, except the sub-lattice deformation in the radial direction, which does not alter the electronic properties of CNTs.

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تغاير تركيب النطاق للأنابيب النانوية الكربونية (SWCNTs) تحت تأثير التشويه الميكانيكي المرن

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الخلاصة:

تمت دراسة الخصائص الإلكترونية للأنابيب النانوية الكربونية الأحادية الجدران (SWCNTs) تحت تأثير عملية التشويه الميكانيكي المرن، وذلك باستخدام تقريب الربط المحكم . في هذا البحث تمت معالجة وتحليل تركيب النطاق للأنابيب النانوية الكربونية الأحادية الجدران (SWCNTs) ضمن مدى واسع من الطاقات حول مستوي طاقة فيرمي. تضمنت الدراسة تطبيق عملية التشويه الأحادي المحور، التدوير الحلزوني وتشويه الشبكة الفرعية، الذي طبق لغرض تحويل خصائص النقل الإلكتروني للأنابيب النانوية الكربونية الأحادية الجدران (SWCNTs)، مثل طيف الطاقة وذلك كدالة لتتصور التشويه الميكانيكي. أظهرت النتائج إن الخصائص الإلكترونية للأنابيب النانوية الكربونية الأحادية الجدران (SWCNTs) تتأثر تحت عمليات التشويه، حيث أن طيف الطاقة يتغير بشكل محسوس نتيجة لذلك.

الكلمات المفتاحية: الأنابيب النانوية الكربونية الأحادية الجدران، (SWCNTs)، تقريب الربط المحكم، طيف الطاقة، فجوة الطاقة، التشويه المرن.