Electronic properties of zigzag and armchair carbon nanotubes under uniaxial strain

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Molecular dynamics simulations and quantum transport theory are employed to study the electronic properties of various zigzag and armchair carbon nanotubes (CNTs) under uniaxial compressive and tensile strains. It is found that the transfer integral decreases as the tensional strain increases. Furthermore, in the $(3N+1,0)$ and $(3N,0)$ zigzag nanotubes, the current induced by the application of a suitable bias voltage varies linearly with the magnitude of the applied strain. Thus, these particular zigzag CNTs are suitable for use as nanoscale strain sensors. Furthermore, the wider detected ranges occur in the smaller diameter of $(3N,0)$ and $(3N+1,0)$ tubes. However, in $(11,0)$ zigzag nanotube and $(5,5)$ armchair nanotube, the variation in current is not in accordance with Ohm’s law with respect to variations in the applied strain. Specifically, the electronic resistance decreases with increasing strain in $(11,0)$ zigzag nanotube, while the current variations in different strains show the irregular and small perturbation in $(5,5)$ armchair nanotube. Accordingly, neither the $(11,0)$ zigzag nanotube nor the $(5,5)$ armchair nanotube is suitable for strain sensing applications, but the $(5,5)$ armchair nanotube has a current with the stable property for a conducting wire.


I. INTRODUCTION

Due to the limited linewidth capabilities of current manufacturing techniques, silicon-based electronic components are basically restricted to conducting wire widths of 60 nm or more. However, nanoscale electronic components consisting of just several atoms or molecules have attracted considerable attention for industrial applications such as tunneling field-effect transistors, single-electron transistors, and so forth in recent years. At such small scales, quantum mechanics principles must be applied to understand the behavior of the system. Carbon nanotubes (CNTs) have emerged as highly promising candidates for the next generation of electronic components, and hence their electronic properties have been extensively studied.1,2 Many reports have attempted to exploit the unique electronic properties of single-walled CNTs (SWCNTs) to develop nanoscale electronic devices. Such nanotubes are no more than several nanometers in diameter and have not only metallic properties but also semiconducting properties, depending on their chiral vector.3

In recent years, various studies have conducted molecular dynamics (MD) simulations to investigate the electronic and mechanical properties of SWCNTs.4,5 In general, the numerical studies show that CNTs possess better mechanical properties than steel, with maximum tensile strains and strengths as high as 30% and 300 GPa, respectively. These high-strength properties render SWCNTs the ideal candidates for use as reinforcement additives in composite material applications. Furthermore, it is shown that the band structures of nanotubes are sensitive to their mechanical deformation. It is found that the energy gap of a nanotube varies as a function of the magnitude of the applied strain.6,7 Furthermore, Umeno et al.8 reported that the electronic properties of SWCNTs change from metallic to semiconducting (and vice versa) as the magnitude of the applied strain increases.

CNT-based detectors have an exciting potential for use in various applications. For example, Kong et al.9 reported that the electronic resistivity of a semiconducting SWCNT undergoes a significant change when it absorbs gaseous molecules such as NO2 or NH3. Furthermore, Ghosh et al.10 indicated that the voltage generated by a SWCNT bundle immersed in a liquid changes with the velocity of the liquid flowing across its surface. Additionally, Dohn et al.11 found that the conductance of multiwalled CNTs (MWCNTs) varies as a function of the applied strain. Meanwhile, Tombler et al.12 reported that the electronic properties of a nanotube vary with the tapping depth in atomic force microscopy applications. Also, several studies have exploited the correlation between the electronic properties of CNTs and their mechanical deformation to fabricate microelectromechanical-system-based microdetectors.13,14

Although the literature contains many experimental investigations related to the feasibility of using CNTs as detectors, very few theoretical studies have been presented. However, numerical simulations can provide valuable insights into the unique features of nanotubes. In our previous study,15 the results suggest that the $(12,0)$ zigzag CNT provides a suitable basis for a uniaxial strain sensor designed to...
detect strain variations in the range of $-0.02$ to $0.16$. Additionally, in the studies investigating the correlation between the energy gap and the tensile strain in zigzag nanotubes,\textsuperscript{6,7} it was found that the variation in the energy gap was dependent on three particular nanotube configurations, namely, (3N,0), (3N−1,0), and (3N+1,0), where N is a positive integer. Furthermore, Minot et al.\textsuperscript{16} showed that tensile strain ($\sigma$) can broaden energy gaps ($E_{\text{gap}}$) in metallic CNTs and one half of semiconducting CNTs, but it can narrow energy gaps down in the other half of semiconducting nanotubes.

According to the above statements, nanodetectors based on nanotubes have an exciting potential for use in a diverse range of applications. However, a lot of calculations merely discuss all kinds of relation between the energy gap and the uniaxial strain. The I-V curves are used more commonly in experiments and provide more information than energy gap does. These results are more suitable and more directly used in the application of strain sensor. Hence, the present study considers eight nanotubes having configurations (3N,0), (3N+1,0), and (3N−1,0) zigzag and (5,5) armchair CNTs to be our models to understand the influence of different chiral vector. Consequently, this study performs MD simulations and quantum transport theory to investigate the transport properties of armchair and zigzag nanotubes under different uniaxial compressive and tensile strains.

**II. CALCULATION DETAILS**

To understand the current-bias voltage (I-V) characteristics of the nanotube under different axial strains, we consider the case of a finite-length CNT attached to either end of an ideal electrode as shown in Fig. 1. In the simulations, the geometric structures and elastic constants of diamond and graphite are modeled using the Tersoff potential\textsuperscript{17} for a carbon atom. This model is a three-body potential function containing an angular term and is commonly used to model the interaction behaviors of C, Si, and Ge. The model of MD simulation distinguishes into two kinds of layers. The atoms in the unit cells located at either end of the nanotube are assumed to be fixed, i.e., they are arranged within a fixed layer, while those in the other unit cells within the nanotube are free to move dynamically, i.e., they are arranged within a free dynamics layer. The velocities of the atoms in the free dynamics layer are scaled using the Berendsen thermostat so that the simulation system converges toward a temperature of 300 K. Each simulation comprises a total of 800 000 time steps, each of which is 0.5 fs, divided into 40 cycles. In each cycle, the first 15 000 time steps maintain a relaxation process, while the remaining 5000 time steps proceed with a deformation process in which the nanotube is compressed or extended in the axial direction by applying a decreasing or an incremental strain rate of $2 \times 10^{-6}$ at each time step. The positions of the atoms within the nanotube are recorded every 100 steps during the final 10 000 time steps of the relaxation process. The bond lengths are then computed based on the average positions of the atoms.

The detailed procedures involved in simulating the electronic properties of a CNT were presented in our previous study.\textsuperscript{18} Briefly, the eigenvalues of the end sites of the semi-infinite metallic electrodes are calculated using the tight-binding method. Subsequently, the interaction between the metallic electrodes and the CNT is evaluated using Dyson equation. The transfer matrix (T-matrix) of the CNT is represented by means of the tight-binding Hamiltonian and the Green’s function. Finally, the current-bias voltage properties of the nanotube are calculated via the Landauer formalism. Here, we only present the Hamiltonian matrix for the tight-binding representation of the armchair nanotube as follows:

$$H_{\text{arm}} = \begin{bmatrix} H_M & H_{t1} & H_{t2} \\ H_{t1} & H_{t2} & H_M \\ H_{t2} & H_M & H_{t2} \end{bmatrix},$$

where this matrix is composed of separate submatrices ($H_M$, $H_{t1}$, and $H_{t2}$), each representing the Hamiltonian of one individual zigzag line parallel to uniaxial direction, $H_M$ represent the zigzag line between the two ends, $t_1$ is the transfer integral in real space, and $H_{t1}$ and $H_{t2}$ represent the transfer integral between adjacent zigzag lines.

The submatrices can be shown as follows:

$$H_M = \begin{bmatrix} E^m + \Sigma_R & t_1 & \cdots \\ t_1 & E^m & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix},$$

$$H_{t1} = \begin{bmatrix} 0 & t_1 & \cdots \\ t_1 & 0 & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix},$$

$$H_{t2} = \begin{bmatrix} 0 & \cdots & t_1 \\ \cdots & \cdots & \cdots \\ t_1 & \cdots & 0 \end{bmatrix}.$$
zigzag and (5,5) armchair CNTs. In a zigzag nanotube, adjacent rings of carbon atoms are referred to as “unit cells” and the interval between them is three times the bond length (a). By contrast, in an armchair nanotube, the interval between two adjacent unit cells is \(\sqrt{3}a\). However, the simulation procedure is similar for both types of nanotube, and hence the following discussions arbitrarily take the case of zigzag nanotubes for illustration purposes. The simulation system for a (10,0) zigzag CNT with length of 93.7 Å contains a total of 880 carbon atoms, equivalent to 22 unit cells.

Previous studies have demonstrated that the energy gap in a nanotube varies according to the extent of the tube’s mechanical deformation.\(^6\)--\(^8\) Furthermore, Dohn et al.\(^11\) reported that the conductance of MWCNTs varies in accordance with the magnitude of the applied strain. Furthermore, it has been shown that in a nanotube subjected to tensile deformation, the transfer integral between two adjacent \(2p_z\) atomic orbitals varies as a function of the bond length.\(^18\) The transfer integral corresponding to any particular value of the bond length is computed by Harrison’s law.\(^18\)

FIG. 2. Variation in transfer integral with applied strain in (10,0) zigzag CNT.

The transfer integral corresponding to any particular value of the bond length is computed by Harrison’s law.\(^18\) Figure 2 presents the variation in the transfer integral with the applied strain for both axial bonds and nonaxial bonds. In general, it is observed that the value of the transfer integral decreases as the tensile strain increases. At strains of less than 0.2, both curves are approximately linear, but it is seen that the transfer integral decreases more rapidly for the axial bonds than for the nonaxial bonds. However, at strains greater than 0.2, the transfer integral remains approximately constant for the axial bonds but decreases significantly for the nonaxial bonds.

This study employs quantum transport theory to investigate the electronic properties of zigzag and armchair CNTs under different strains. In general, all armchair nanotubes \((n,n)\) have metallic properties. However, zigzag nanotubes \((n,0)\) are metallic only when the index \(n\) is a multiple of 3. In other words, approximately one-third of zigzag nanotubes are metallic, while two-thirds are semiconductors. The zigzag nanotubes considered in the present simulations vary in length from 24.5 to 85 Å, equivalent to 6–20 unit cells, respectively. The chemical energies of the left and right electrodes are denoted as \(\mu_1\) and \(\mu_2\), respectively, and an assumption is made that the tunneling transport mechanism in the arrangement shown in Fig. 1 is coherent. As stated previously, the metallic electrodes are assumed to be semi-infinite chains and are attached to the nanotube via a weak coupling between the atoms at the interface of the electrodes and the side heads of the nanotube. Finally, the simulations are based on a tight-binding interaction Hamiltonian.

In the simulations, the coupling between the nanotube and the electrodes \((V_e)\) is assumed to have a value of 0.4 eV, for instance, the coupling between two Ti and each of the six C neighbors is about 0.3 eV.\(^15\) Furthermore, the bandwidth of the electrodes \((V_e)\) is 16.0 eV, and the transfer integral of the CNT \((t_0)\) is assigned to a value of \(-3.033\) eV at strain of 0. In a practical application, the bias voltage applied to the arrangement shown in Fig. 1 is distributed in accordance with a ratio \(\kappa\), with a voltage of \(\kappa V\) applied to the left electrode and a voltage of \(-(1-\kappa)V\) applied to the right. However, for simplicity, the current simulations assume that the bias applied to the electrodes has a symmetrical distribution, i.e., \(\kappa=0.5\), and suffers no dissipation in contact. In other words, the biases applied to the left and right electrodes are \(+V/2\) and \(-V/2\), respectively.

FIG. 3. Variation in current with bias voltage in zigzag and armchair CNTs of different lengths. (a) I-V profiles in (10,0) zigzag CNTs, (b) I-V profiles in (12,0) zigzag CNTs, and (c) I-V profiles in (5,5) armchair CNTs.
responds to the bias voltage required to shift the electrons from one discrete energy state to another. Under these conditions, the electrons drift between the two electrodes and a current is generated in the nanotube. It can be seen that the number of steps in the current-voltage profile increases with the nanotube length. In a shorter tube, the quantum effect results in the energy level being made up of discrete energy states. However, in tubes with a length of several hundred nanometers or so, the energy level has a quasicontinuous characteristic, and hence the height of the step feature reduces, giving the curve a smoother appearance. In the nanotube/electrode arrangement shown in Fig. 1, the length of the nanotube (that is below 200 nm) is much shorter than that of the mean free path (1.6 μm), and in this way, the conductor is called ballistic conductor. Under the circumstances, electrons are conducted through the nanotube without scattering and encounter zero electronic resistance. However, they encounter a resistance when they arrive at the contact between the nanotube and the electrodes. Therefore, the resistance within the nanotube/electrode assembly is independent of the nanotube length and varies only as a function of the number of transverse modes in the lead. Figure 3(a) shows that the current is close to zero when bias voltages are lower than 1.1 V [i.e., the energy gap of the (10,0) nanotube] with lengths of 12 and 20 unit cells. This leakage current is a result of the tunneling effect in a length of 6 unit cells. It is apparent that the tunneling effect becomes less severe as the length of the nanotube increases. Figures 3(b) and 3(c) show that the currents are close to zero for very low bias voltages in the (12,0) zigzag and (5,5) armchair nanotubes with a length of 20 unit cells, respectively. These results reflect the fact that (12,0) zigzag and (5,5) armchair nanotubes are zero-gap semiconductor and metal, respectively. But the tubes with shorter length are affected by the Coulomb block effect and the discrete energy states, so only at the higher voltage does the current appear little by little. In general, it can be seen that the curves of nanotubes with different lengths have the same trend and have influence only on the number of the steps, and hence it is inferred that the size effect has only little influence on the I-V characteristics. Accordingly, nanotubes with a length of 20 unit cells are chosen as the basis for the following strain simulation model.

To clarify the effects of strain on the current flow within the nanotube, Fig. 4 illustrates the current-bias voltage profiles of a (10,0) zigzag nanotube at uniaxial strain (both compressive and tensile). As shown in Fig. 4(a), at bias voltages lower than 2.5 V, the current increases and the energy gap decreases with increasing compressive strain. The current variation arises from the compressed tube and thus causes the transfer integral variation. However, the energy gap increases with the magnitude of the increasing tensile strain, as shown in Fig. 4(b). In Fig. 4(c), it is seen that the current-voltage profiles corresponding to different values of applied strain are virtually superimposed with one another, but the energy gap gradually reduces as the strain is increased beyond 0.06. As shown in Figs. 4(b) and 4(c), the current-voltage profiles are superimposed with one another at bias voltages higher than 2 V. Furthermore, it is apparent that in (10,0) zigzag nanotubes, the profiles are interleaved with one another at lower bias voltages as the tensile strain is increased. A similar phenomenon was reported for metal zigzag nanotubes by Yang and Han, who observed that the lowest energy band near the Fermi energy broadened when the nanotube was subjected to a tensile strain, while the second lowest energy band narrowed.

Figure 5 shows the profiles of electronic current of the (11,0) zigzag nanotube versus bias voltage under different strains. In Fig. 5(a), the profile characteristics are precisely opposite of those observed in Fig. 4(a), i.e., the current decreases and the energy gap increases with increasing compressive strain. Conversely, Fig. 5(b) shows that the current increases and the energy gap decreases as the magnitude of the tensile strain is increased. Furthermore, it is observed that the current-voltage profiles are unevenly spaced as the tensile strain is increased. Although the relationship between the
transfer integral and the strain is similar in the (10,0) and (11,0) nanotubes, it is evident that the strain-dependent characteristics of the current-voltage relationships of the two zigzag nanotubes are quite different in Figs. 4 and 5. In general, the electronic resistance obeys Ohm’s law $[R = \sigma L / A]$ in mesoscopic conductors. As the strain increases, the length ($L$) of the nanotube also increases and the cross-sectional area ($A$) decreases. Hence, the electronic resistance increases (current decreases) and energy gap increases with increasing tensile strain in the (10,0) nanotube. However, the opposite trend is observed in the (11,0) zigzag nanotube. These opposite phenomena occur when the tube is subjected to a tensile strain because the lower energy band leaves Fermi energy in the (10,0) and (12,0) nanotubes and approaches Fermi energy in (11,0) tube. The previous studies also find the similar phenomena that the energy gap increases in $(3N + 1,0)$ and $(3N,0)$ zigzag tubes but it decreases in $(3N - 1,0)$ zigzag tube under the tensile strains. In addition, Minot $et al.$ showed that the resistance decreases and conductance increases with increasing tensile strain in semiconductor CNT. The variation in the current versus the applied bias voltage under different strains in (12,0) zigzag nanotube was presented in our previous study, so the figures are not shown here again.

Figure 6 shows the variation in the current with the applied bias voltage at different strains in (5,5) armchair nanotube. Figure 6(a) shows that the profiles associated with higher values of compressive strain are interlaced with those corresponding to lower compressive strains. Furthermore, it can be seen that, at voltages lower than 0.4 V, the maximum current is obtained at compressive strains of −0.02 to −0.03 in Fig. 6(a) and the minimum current is produced at tensile strains of 0.02 in Fig. 6(b). In general, it is observed that the current variations at different strains only perturb slightly and change irregularly. This is because the lower energy band slightly deforms when the (5,5) armchair nanotube was subjected to the compressive and tensile strains. Hence, the armchair nanotube always has metallic property under the compressive and tensile strains.

The normalized current-strain profile could be gained by the variation in current with applied bias voltage (Figs. 4–6). Figures 7 and 8 plot the profiles of normalized current with strain for different applied bias voltages in zigzag and armchair nanotubes. Note that in the figure, the current is normalized by dividing the actual current at different strains ($I$) by the reference current ($I_0$), i.e., the current is obtained under zero strain conditions. As shown in Fig. 7(a), corresponding to the (10,0) zigzag tube, the current-strain profiles have a linear characteristic for strains ranging from −0.05 to +0.06 for bias voltages of 1.6–1.8 V. Under these conditions, the
normalized current varies from approximately 0.2 to 2.1. It is also observed that under a tensile strain, the current is more sensitive to changes in strain at lower bias voltages. In general, the results indicate that the (10,0) nanotube is suitable for strain detection purposes over the strain range of −0.05 to +0.06. Figure 7(f) shows the variation in the normalized current with the strain for different applied bias voltages in (12,0) metallic zigzag nanotube. The figure shows that the maximum normalized current is obtained at compressive strain of −0.03. However, as the nanotube is subjected to an increasing tensile strain, the current decreases. In this sense, the results are consistent with those observed in the (10,0) nanotube shown in Fig. 7(a). In the case of the (12,0) nanotube, Fig. 7(f) shows that the normalized current-strain profiles have a linear form at the strain range of −0.02 to +0.10 for bias voltages between 1.0 and 1.8 V. Under these conditions, the normalized current varies ranging from approximately 0 to 2.5. Furthermore, under both compressive and tensile strains, the sensitivity of the current to changes in the strain is enhanced at lower bias voltages. Hence, the results show that the (12,0) nanotube is suitable for the detection of strains lower than 0.16.

According to the above results, the (10,0) and (12,0) zigzag nanotubes are both suitable for strain sensing applications. Some questions about whether the other (3N+1) and (3N,0) zigzag tubes have the same property exist. Due to this doubt, following a similar procedure used before, we plot the profiles of the normalized current with strain for different applied bias voltages in (9,0), (13,0), (15,0), and (16,0) zigzag tubes, as shown in Fig. 7. The current-strain profiles of (3N+1) zigzag tubes show the same trends in Figs. 7(a)–7(c). In addition, the profiles have the wider linear range at the bias voltages of 1.8, 1.3, and 1.1 V in (10,0), (13,0), and (16,0) tubes, respectively. Hence, the results show that the line relationships between strain and normalized current not only appear at the lower bias voltage but also reduce the detected range with increasing diameter (increasing number N). By observing Figs. 7(d)–7(f), we find that the current-strain profiles have the maximum detected strains of 0.17, 0.16, and 0.13 in (9,0), (12,0), and (15,0) tubes, respectively. In this way, the results show that the line relationships in strain-current profiles appear at the lower bias voltage and restrict the detected range with increasing diameter (the increasing number N) in those figures in (3N) zigzag tubes. In the result mentioned above, the wider detected ranges occur at the lower bias voltage and the ranges reduce with increasing diameter in the group of (3N,0) and (3N+1,0) tubes.

Figure 8(a) shows the variation in the normalized current with the strain for different applied bias voltages in (11,0) zigzag nanotube. In Fig. 8(a), the slopes of the profile are a positive (+) number (i.e., the current increases with increasing tensile strain), which are different from those observed in Fig. 7(a). Furthermore, it is observed that the current-strain profiles have no linear relations as the compressive and tensile strains increase, and the normalized current under the strain of 0.08 even becomes eight times as strong as the current obtained under zero strain. Figure 8(b) shows the variation in the normalized current with the strain for different applied bias voltages in (5,5) armchair nanotube. The figure also shows that the normalized current at different strains only perturbs slightly and changes irregularly, and thus, the armchair nanotube is unsuitable for strain sensing applications. However, the normalized current varies merely ranging from approximately 0.87 to 1.05, and the current variation is smaller than that in the other zigzag nanotubes. Hence, the current variation in the armchair nanotube is more stable under small uniaxial strains, and this characteristic could be applied to thermal strain. When a conducting wire needs a stable current and is slightly affected by small strain, the armchair tube is a very suitable choice.

However, the current-strain profiles have two different trends in these three zigzag tubes. The current decreases with increasing tensile strain in (10,0) and (12,0) tubes but increases with increasing tensile strain in (11,0) tubes. The appearance of things is due to the density of states (DOS) which could be shifted and deformed under strain, and the similar phenomena appear in Ref. 6. In the previous study, the peak that is closest to Fermi level leaves the Fermi level in (3N,0) and (3N+1,0) tubes, and thus the gaps become broad gradually and the current decreases as the tensile strain increases. On the contrary, the nearest peak approaches the Fermi level in (3N−1,0) tube, making the gaps become narrow gradually and the current increase with increasing tensile strain. Finally, the variations in DOS cause two different trends in current-strain profiles.

The results presented in Fig. 7 suggest that (3N+1,0) and (3N,0) zigzag nanotubes are both suitable for strain sensing applications. Hence, this relationship between the scaled current (S) and the strain of the tube (ε) can be defined as a linear equation, $S = 1 - m(V)ε$, and $m$ is a factor which changes with the voltage (V). For example, the equation can be written as $S = 1 - 11.0ε$ at the bias voltage of 1.8 V in Fig. 7(a). In other words, the elongation of tube strain is 5%, and the variation in the current decreases by 55%. In general, the application of a uniaxial strain to a nanotube induces a change in the tube’s bond length. This in turn causes a change in the transfer integral of the tube and hence prompts a change in its DOS. Therefore, if the nanotube is suitably biased, a measurable change in the current is observed. Figures 7(a)–7(c) show that (3N+1,0) zigzag nanotubes are capable of detecting compressive strains between −0.05 and +0.05. Therefore, the (3N+1,0) nanotubes are suitable for strain sensing applications in which the strain can act in either a compressive or a tensile direction, and the (3N,0) nanotube are suitable for strain sensing applications in large tensile strains. Meanwhile, Figs. 7(d)–7(f) show that the variations in the (3N,0) zigzag tubes are more sensitive to that of the strain at lower applied bias voltages but have the more restricted strain measurement range. Accordingly, the nanotubes are particularly suitable for strain detection applications in which the strain variation is known to be small. Furthermore, the maximum detected ranges occur at the lower bias voltage and reduce with increasing diameter of (3N,0) and (3N+1,0) tubes. The results presented for the (11,0) tube in Fig. 8(a) have shown that the electronic resistance does not obey Ohm’s law. Furthermore, in a (5,5) armchair nanotube, Fig. 8(b) shows that the current variation at
different strains has irregular and slight perturbations. Therefore, neither the (11,0) nanotube nor the (5,5) nanotube is suitable for strain sensing applications, but the (5,5) armchair nanotube is a very suitable choice for a stable conducting wire. Overall, the normalized current with the uniaxial strain exhibits three quite distinct trends in the current zigzag and armchair nanotubes. However, these three distinct trends have not been found in several previous experiments in which the models are MWCNTs (Ref. 11) or nanotube film based on SWCNTs.\textsuperscript{21} When the MWCNT contains a layer of metallic CNT or SWCNT film contains several percent of metallic CNTs, their electronic properties possess metallic properties and do not show the semiconductor properties. Additionally, these properties of the normalized current in MWCNT or SWCNT film include the interactions of SWCNTs, so the trends of individual SWCNT are different from those of MWCNT or SWCNT film.

IV. CONCLUSIONS

This study has performed a theoretical investigation into the electronic properties of zigzag and armchair nanotubes under uniaxial compressive and tensile strains. In general, the results have shown that the current-bias voltage profiles are characterized by distinct steps at particular values of the bias voltage. These steps correspond to the bias voltage at which the electrons imparted sufficient energy to propagate through the nanotube. The simulation results have also shown that the value of the transfer integral decreases as the magnitude of the tensile strain increases. In (3N+1,0) and (3N,0) zigzag nanotubes, the change in the current induced in the nanotube by the applied bias voltage is linearly related to the variation in the applied strain. Therefore, these particular nanotubes are suitable for nanoscale strain sensing applications. Specifically, the (3N+1,0) zigzag nanotubes are suitable for detecting compressive and tensile strains—i.e., $-0.05 \rightarrow +0.05$—while (3N,0) zigzag CNTs are suitable for detecting a high strain rate detection capability—i.e., $-0.03 \rightarrow +0.12$. Furthermore, the maximum detected ranges occur at the lower bias voltage and reduce with increasing diameter of (3N,0) and (3N+1,0) tubes. Finally, in the (11,0) zigzag nanotube and the (5,5) armchair nanotube, the variation in the current does not obey Ohm’s law related to the variation in the applied strain. Specifically, the resistance decreases and the current increases with increasing tensional strain in the (11,0) zigzag nanotube, while the current variations at different strains only have irregular and slight perturbations in the (5,5) armchair nanotube. Overall, the simulation results show that the normalized current with the strain exhibits three quite distinct trends in the current zigzag and armchair nanotubes.

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