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RESEARCH PAPER

The Effect of Compressive Stress and Tensile Strain on Graphene Nanoribbon Island in Single Electron Transistor

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ABSTRACT

The single electron transistor (SET) is nanoscale device that can be utilized in future integrated circuits. It contains three electrodes and one island that is located between them. The island material impacts on SET performance. Therefore graphene with unique properties is selected for the island material with compressive stress and tensile strain imposed on it. In this paper, an appropriate mathematical model is derived for the device current taking the impact of compressive stress and tensile strain on the graphene nanoribbon (GNR) island into account. Moreover, the impact of numbers of atoms along the GNR length and applied gate voltage are investigated and the obtained I-V curves are compared together. Furthermore, the SETs island are designed and their band structures are plotted and then their band gaps are calculated. The charge stability diagrams of SET with compressive stress and tensile strain are plotted and analyzed. Their coulomb diamond areas and coulomb blockade ranges are compared together. Finally, GNR SET with better operation is defined.

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INTRODUCTION

The semiconductor industry needs to small size transistors [1]. Moore's law expresses increasing transistors with passing time in each chip [2]. Therefore scaling transistor goes toward nanoscale [3,4]. The single electron transistor (SET) is a nanoscale transistor which its channel has nanometer size [5]. Some SETs are designed and fabricated for IC such as Hybrid CMOS-SET analog IC and IC-Oriented Si SETs [6,7]. The SET structure contains an island which locates in SET channel [8]. The single electron can tunnel to SET island through tunnel barrier when Fermi energy source is lower than first unoccupied energy level in island (The tunnel barrier contains a capacitor and a resistance). Then this electron tunnels to drain electrode and current flows in SET [9]. Quantum dot materials such as graphene nanoribbon (GNR) can be utilized in island of SET [10,11,12]. Graphene is a carbon based material and has unique properties such as high electron mobility. It's mobility is higher than some materials mobility which can utilize as island SET [13]. The distance between neighboring carbon atoms in GNR is 1.42 which can be changed due to applied compressive stress and tensile strain on GNR [14]. The compressive stress and tensile strain of GNR can be engineered [15,16]. The impact of compressive stress and tensile strain on the distance between neighboring carbon atoms

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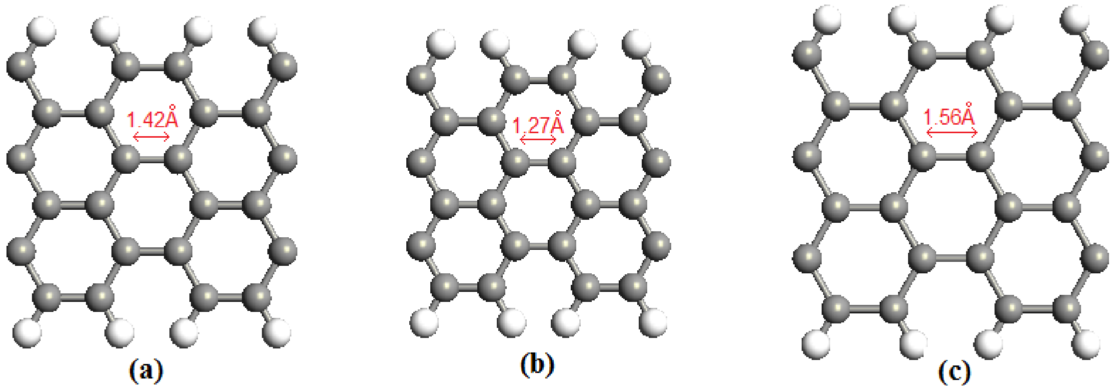


Fig. 1. (a) Graphene nanoribbon (GNR) in equilibrium. (b) GNR with comparative stress of %10 Pa. (c) GNR with tensile strain of %10 Pa.

in GNR are shown in Fig. 1 [17].

The compressive stress decreases carbon-carbon bond length but the tensile strain increases this bond length [18]. The changing bond and distance between carbon atoms affect on properties of GNR and consequently SET performance and its current [19]. In this research, a mathematical model for the SET current with compressive stress and tensile strain on GNR island is derived and then implemented utilizing MATLAB software. The effect of some parameters such as value of compressive stress and tensile strain on GNR island, number of carbon atoms along the GNR and applied gate voltage on the SET current will be investigated. The charge stability diagrams of GNR with different values of compressive stress and tensile strain on GNR will be derived with the aid of Atomistix ToolKit (ATK) software and they will be compared together. Finally, the best island for utilizing in the SET will be defined.

Mathematical model of current considering compressive stress and tensile strain on GNR island SET

The SET contains three electrodes and an island between them [20]. The mathematical model is written for SET current based on solving Schrödinger equations. The different parts of SET are shown in Fig. 2 which is essential for deriving of a mathematical current model [17].

The SET contains an island as a potential well and two tunnel junctions as tunnel barriers which are shown in Fig. 2. The electron wave functions derived from the Schrödinger equations in different regions of the device are given in the following [21].

$$\Psi_I = A_1 e^{k_1 x} + B_1\, e^{-k_1 x} \tag{1}$$

$$\Psi_{II} = A_2 e^{ik_2 x} + B_2\, e^{-ik_2 x} \tag{2}$$

$$\Psi_{III} = A_3 e^{ik_3 x} \tag{3}$$

where $k_1 = k_3 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$ and $k_2 = \frac{\sqrt{2mE}}{\hbar}$

The above equations can be solved considering the associated boundary conditions as:

$$\Psi_I(0) = \Psi_{II}(0) = A_1 + B_1 = A_2 + B_2 \tag{4}$$

$$\Psi_I{}'(0) = \Psi_{II}{}'(0) = ik_1 A_1 - ik_1 B_1 = k_2 A_2 - k_2 B_2 \tag{5}$$

$$\Psi_{II}(\mathrm{L}) = \Psi_{III}(\mathrm{L}) = A_2 e^{k_2 L} + B_2\, e^{-k_2 L} = A_3 e^{-ik_1 L} \tag{6}$$

$$\Psi_{II}{}'(L) = \Psi_{III}{}'(L) = k_2 A_2 e^{k_2 L} - k_2 B_2\, e^{-k_2 L} = ik_1 A_3 e^{ik_1 L} \tag{7}$$

Then the electron transmission coefficient of the GNR SET can be calculated as eq. 8 [22].

where K_B is Boltzmann's constant, T is the temperature, $x = E\text{-}E_g / K_B T$, E is energy, E_g is band

$$T = \frac{[(K_B T)^2 x + \left(\frac{1.04}{w}\right)]}{([(K_B T)^2 x + \left(\frac{1.04}{w}\right)] + [K_B T x + \left(\frac{1.04}{w}\right) + K_B T x]^2 + (L^2\left[K_B T x + \left(\frac{1.04}{w}\right)\right])^{0.5} + [\left(L^2\left[K_B T x + \left(\frac{1.04}{w}\right)\right]\right)/6]^{1.5})^2} \tag{8}$$

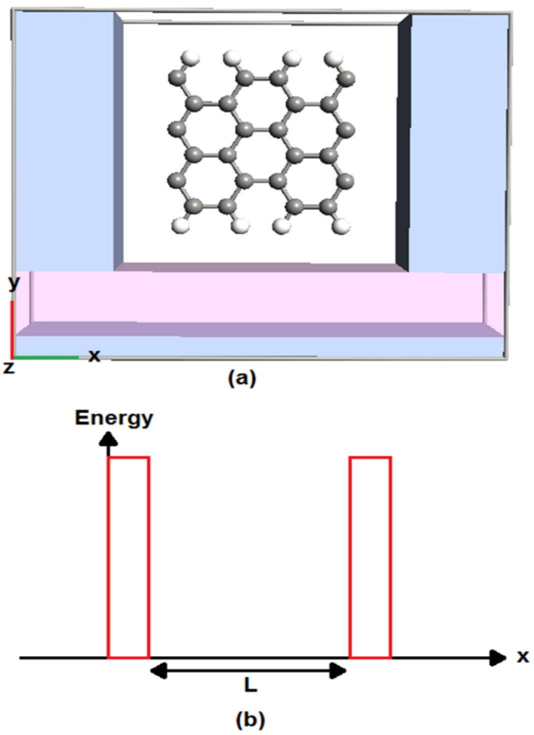


Fig. 2.(a) Graphene nanoribbon SET. (b) The energy profile vs channel length which indicates SET island as a quantum well.

gap energy, *w* is GNR width and *L* is GNR length. The Landauer formalism can be utilized for modelling of the current as:

$$I = \int_0^{\eta} T(E).F(E)dE \quad (9)$$

$$\mathrm{w} = 0.866(N_2 - 1)(1 + Z)a_{c-c} \quad (10)$$

where T(E) is the transmission coefficient of the electrons and F(E) is the Fermi function or occupation probability, $\eta = E_F - E_g / K_B T$ and E_F is Fermi level energy.

The GNR Length and GNR width are calculated based on number of carbon atoms and value of compressive stress and tensile strain in GNR as

$$\mathrm{w} = 0.866(N_2 - 1)(1 + Z)a_{c-c} \quad (11)$$

$$\mathrm{L} = ([(1.5N_1 - 1)(1 + \mathrm{Z})a_{c-c}]^2) \quad (12)$$

where N_1 is the number of atoms in GNR length, N_2 is the number of atoms in GNR width, *Z* is the value of compressive stress and tensile strain in GNR and a_{c-c} is carbon to carbon bond length in equilibrium which equals 1.42 Å.

The Landauer formalism is utilized for modelling of current SET that SET island is GNR with compressive stress and tensile strain. This mathematical model of current SET is written as eq. 13.

The parameters are defined previously.

The current of GNR SET with compressive stress and tensile strain on GNR island is investigated based on the proposed model. The different

$$I = \int_0^{\eta} [(K_B T)^2 x + \left(\frac{1.04}{0.866(N2-1)(1+Z)a_{c-c}}\right)]([(K_B T)^2 x + \left(\frac{1.04}{0.866(N2-1)(1+Z)a_{c-c}}\right)] + [K_B T x + \left(\frac{1.04}{0.866(N2-1)(1+Z)a_{c-c}}\right) + K_B T x]^2 + ([(1.5\mathrm{N}1 - 1)(1 + \mathrm{Z})a_{c-c}]^2 \left[K_B T x + \left(\frac{1.04}{0.866(N2-1)(1+Z)a_{c-c}}\right)\right])^{0.5} + [\left([(1.5\mathrm{N}1 - 1)(1 + \mathrm{Z})a_{c-c}]^2 \left[K_B T x + \left(\frac{1.04}{0.866(N2-1)(1+Z)a_{c-c}}\right)\right]\right)/6]^{1.5})^{-2} . \frac{dE}{1+e^{x-\eta}} \quad (13)$$

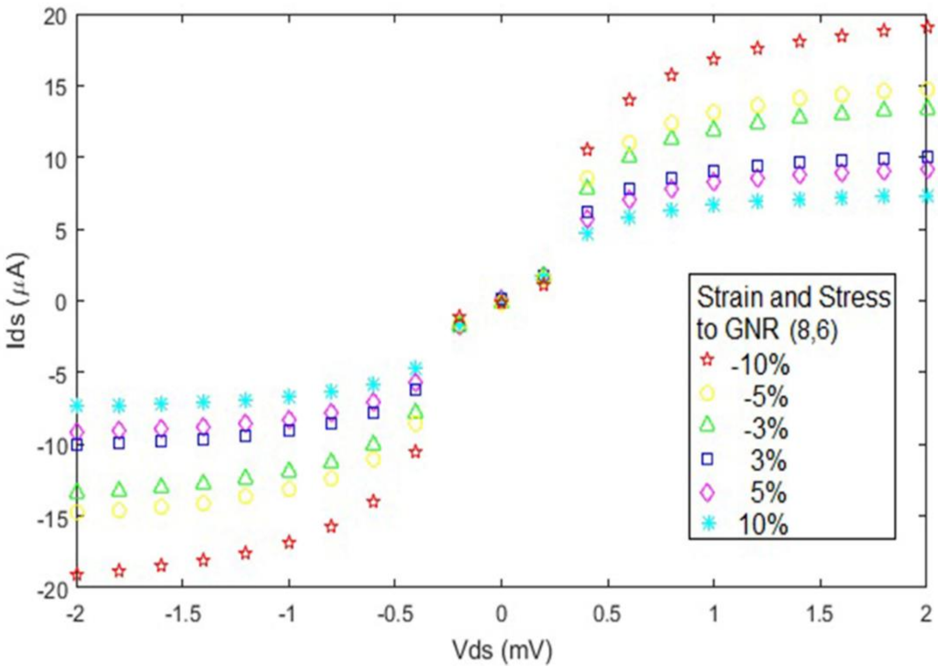


Fig. 3. The current vs. voltage diagram obtained from the proposed model for different value of compressive stresses and tensile strains on GNR island at 300 °K and Vgs is 1V.

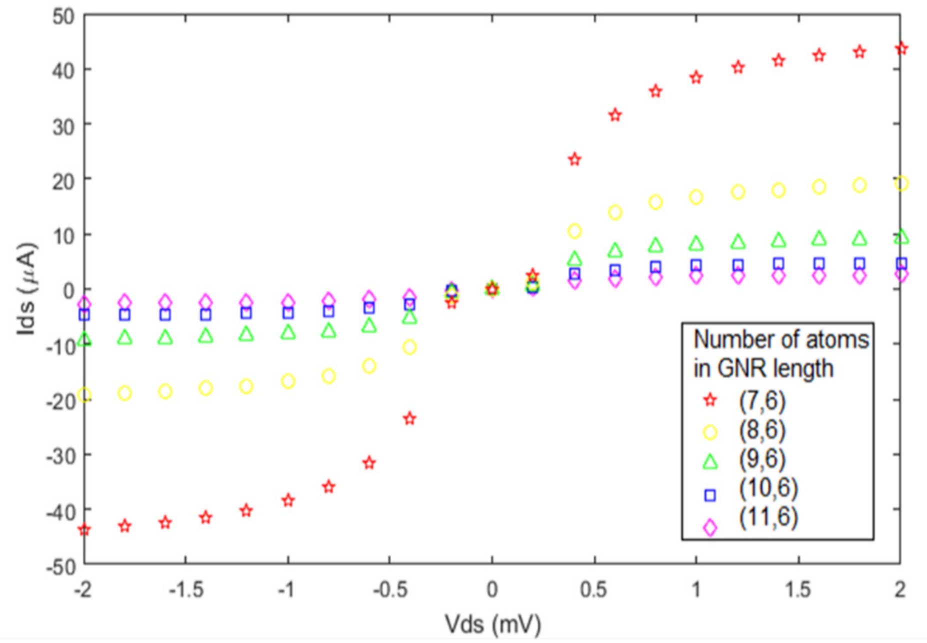
values of compressive stress and tensile strain are applied to GNR island and the obtained results are shown in Fig. 3.

In the analysis performed in Fig. 3, compressive stress changes from -3% to -10% and tensile strain varies from 3% to 10%. The highest current is seen for compressive stress -10% because it has lower carbon bond length and island area. The decreasing carbon bond length decreases quantum well length. Therefore, speed of electron transfer in island will be increased and SET current will be raised. The impact of different number of carbon atoms in GNR length with an applied compressive stress and tensile stress of 0.1Pa to GNR island is investigated and illustrated in Fig. 4.

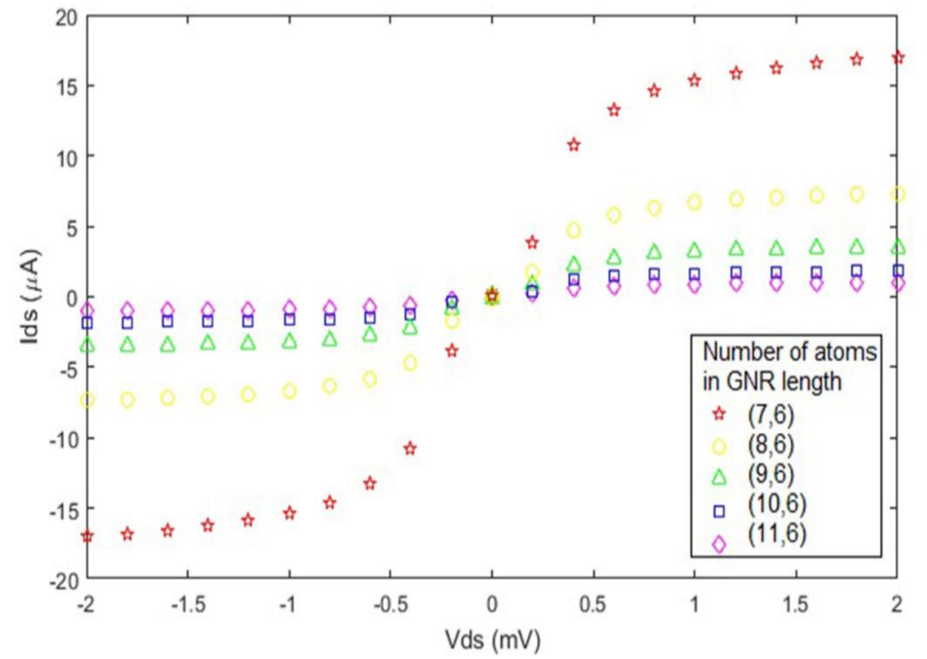
The curves inside Fig. 4(a) indicate that compressive stress on GNR with lower numbers of atoms along the GNR length produces higher current and lower coulomb blockade range. The zero current region in the device with more atoms along the GNR length is higher, i.e. for the (11,6) device. As a result, Fig. 4(a) indicates that the number of atoms along the GNR length has a direct impact on the device current while a compressive stress is applied to GNR. Moreover, The analysis of Fig. 4(b) verifies that decreasing numbers of atoms in GNR length can increase SET current. The physical reason of this current behavior is similar to that explained in Fig. 4(a). However, the comparison of Fig. 4(a) and Fig. 4(b) reveals the fact that increasing the number of atoms along the island length has more impact in the case of compressive stress rather than tensile strain with the same amount. In other words, current has higher value in GNR SET with compressive stress than tensile strain.

The applied gate voltage is another factor which has impact on the SET current. Therefore GNR with 8 carbon atoms in it’s length and 6 carbon atoms in it’s width is selected for SET island. Moreover the compressive stress 0.1Pa and tensile strain of 0.1Pa are applied to this island. The current – voltage curves are plotted in Fig. 5 for different applied gate voltages to these GNR SETs.

The analysis of Fig. 5 indicates that increasing of the applied gate voltage rises SET current. This is due to the fact that a higher gate voltage decreases island’s energy level and then an unoccupied energy level locates in the transfer window. Therefore an electron can tunnel faster and charge flows at a higher speed in SET. The coulomb blockade range also decreases in higher applied gate voltages. Comparison of the obtained results from Fig. 5(a) and Fig. 5(b) indicates that

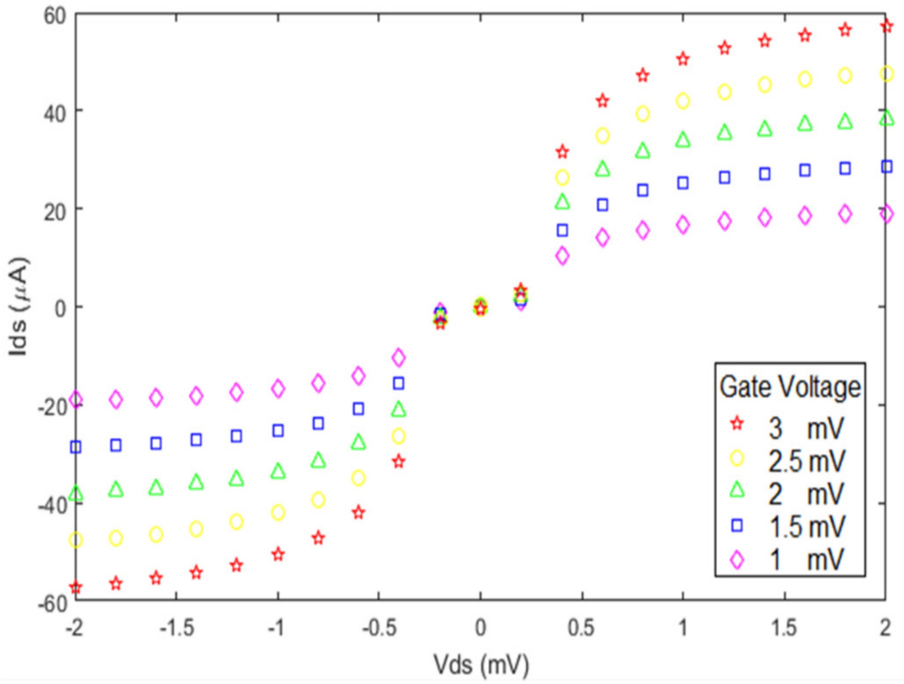


(a)

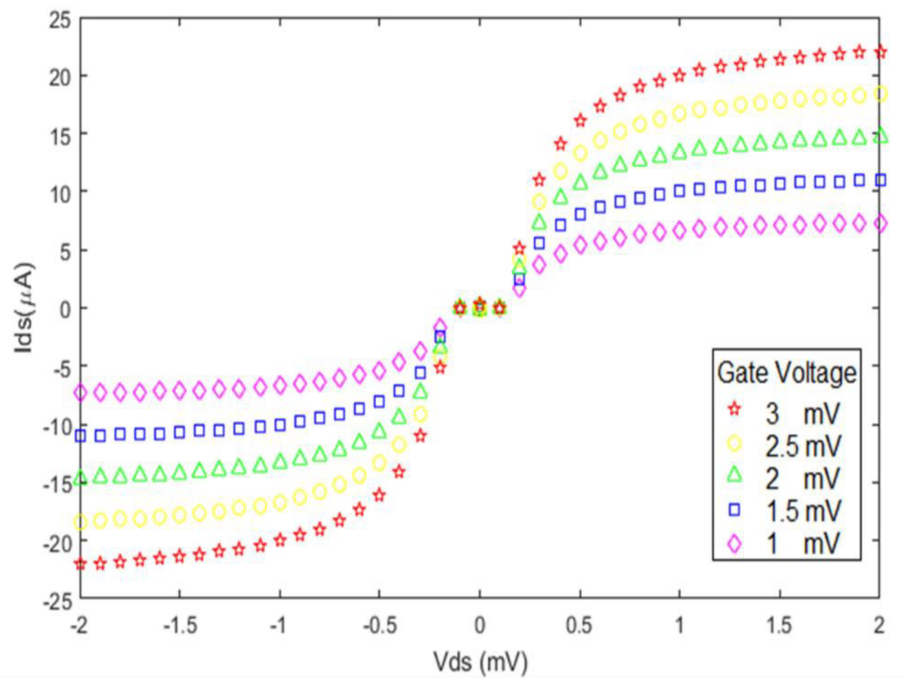


(b)

Fig. 4. The current vs. voltage diagram obtained from the proposed model for different number of atoms along the length of the island, 6 atoms assumed along the GNR width; (a) for an applied compressive stress of 0.1Pa to the island, (b) for an applied tensile strain of 0.1Pa to the island and Vgs is 1V.



(a)



(b)

Fig. 5. The current vs. voltage diagram obtained from the proposed model for different applied gate voltages to GNR SET (8,6); (a) for an applied compressive stress of 0.1Pa to the island. (b) for an applied tensile strain of 0.1Pa to the island.

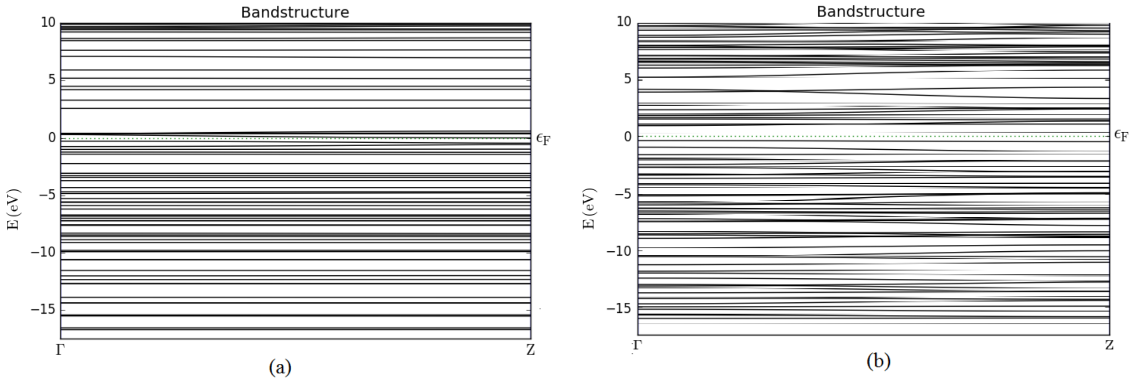


Fig. 6. The band structures of GNR with 24 carbon atoms (a) GNR band structure with compressive stress of %10Pa on the island. (b) GNR band structure with tensile strain of %10Pa on the island.

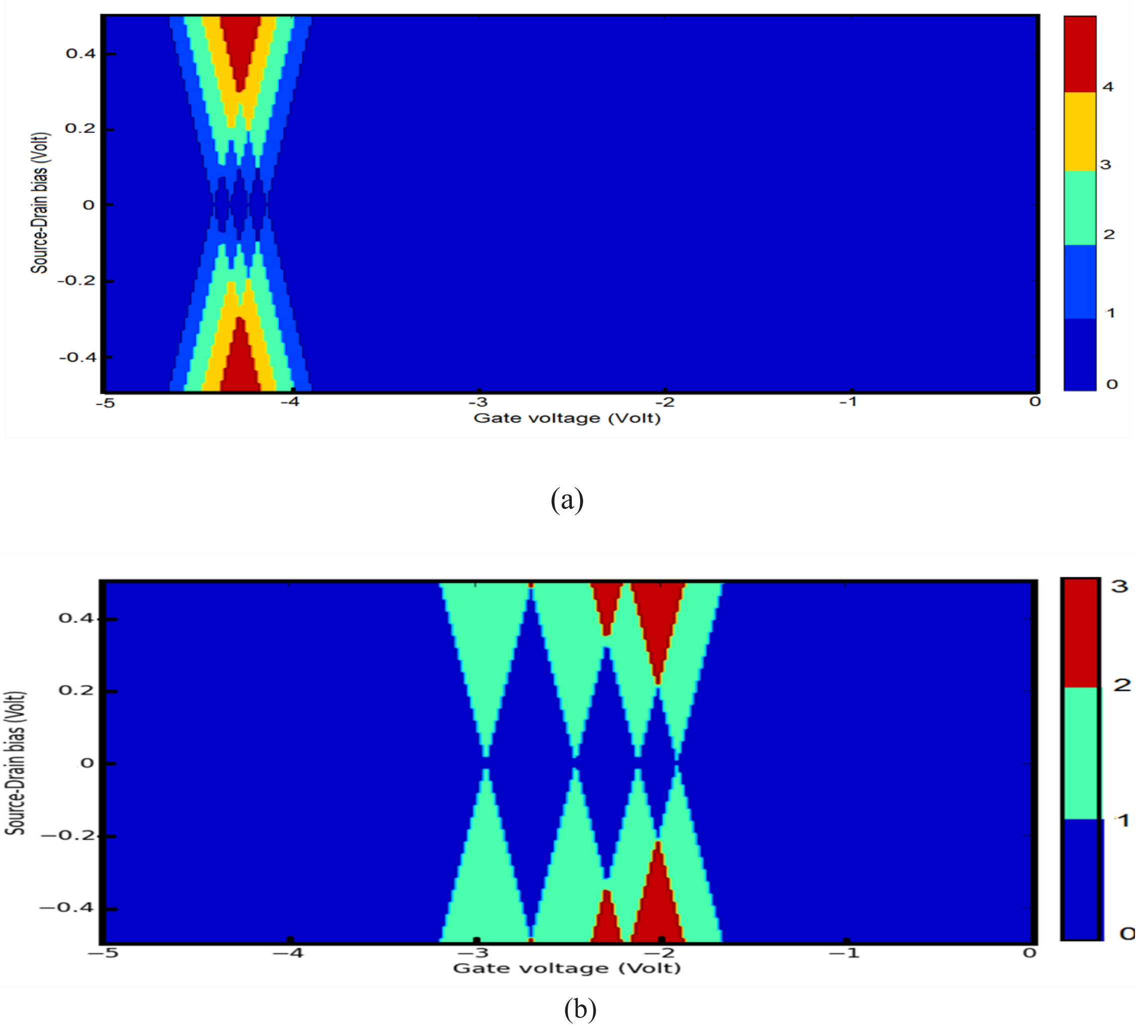


Fig. 7. The charge stability diagrams of GNR SET (a) $V_g - V_{ds}$ with compressive stress of %10Pa on the island. (b) $V_g - V_{ds}$ with tensile strain of %10Pa on the island. (The color bar on the right represents the corresponding charge states in the diagram).

Table 1. Some parameters extracted form charge stability diagrams in Fig.7.

Type of SET	Diamond	$V_{g_{min}}$ (v), $V_{g_{max}}$ (v)	ΔV_g(v)	$V_{ds_{min}}$(v), $V_{ds_{max}}$ (v)	ΔV_{ds}(v)	Diamond Area (v)	Total Diamonds Areas(v^2)
GNR SET with compressive stress of -%10Pa on the island	diamond 1	(-4.417,-4.329)	0.088	(-0.088,0.088)	0.176	0.007	
	diamond 2	(-4.327,-4.228)	0.099	(-0.101,0.099)	0.20	0.009	0.024
	diamond 3	(-4.226,-4.134)	0.092	(-0.097,0.097)	0.194	0.008	
GNR SET with tensile strain of +%10Pa on the island	diamond 1	(-2.931,-2.450)	0.481	(-0.479,0.477)	0.956	0.229	
	diamond 2	(-2.448,-2.120)	0.328	(-0.331,0.334)	0.665	0.109	0.382
	diamond 3	(-2.120,-1.906)	0.214	(-0.208,0.210)	0.418	0.044	

increasing of applied gate voltage has more significant impact on the current of the SET device with a compressive stress of 0.1Pa than the counterpart device with equal amount of tensile strain on the island.

The band structures and charge stability diagrams considering compressive stress and tensile strain on GNR island SET

The single electron transistor can work in low voltage bias [23]. The GNR SETs with 24 carbon atoms are designed with Atomistix ToolKit (ATK) software [17]. Then compressive stress and tensile strain are applied on GNR island and they effect on all carbon-carbon bonds of GNR and all bonds length are equal together. The carbon - carbon bond of GNR with compressive stress of %10Pa is 1.27 and the carbon - carbon bond of GNR with tensile strain of %10Pa is 1.56 . The band structures are plotted in Fig. 6 to evaluate the effects of compressive stress and tensile strain on GNR band gap.

The analysis of band structures of GNR with compressive stress of %10Pa and tensile strain of %10Pa are shown that band gap value of GNR with compressive stress of %10Pa is 0.578 eV and band gap value of GNR with tensile strain of %10Pa is 0.659 eV.The comparison study indicates that the band gap of island with compressive stress is lower than island with tensile strain. Therefore electron transfer in GNR with compressive stress has higher speed and lower zero current range. The electron transfer stops in SET when coulomb blocked phenomena occurs [24]. The coulomb blocked conditions occur when the island charge is higher than the bias voltage, the thermal energy is higher than the charging energy and the tunneling resistance becomes less than 25813Ω. The charge stability diagram shows coulomb blockade range as coulomb diamonds. These diagrams are examined and plotted with the aid of Atomistix Toolkit (ATK) software that DFT method using local-density approximation (LDA) is selected for simulations [17]. The simulations are done for compressive stress of %10Pa and tensile strain of the same amount on the GNR island. These charge stability diagrams are plotted in Fig. 7.

The coulomb blockade ranges are shown in Fig. 5 and coulomb diamonds in charge stability diagrams are shown in Fig. 7. some parameters are extracted from Fig. 7 as presented in Table 1 to evaluate the coulomb blockade ranges and coulomb diamonds area in GNR SET with the same amount of compressive stress and tensile strain on the island.

The comparison of data given in Table.1 indicates that compressive stress and tensile strain on the GNR island impacts on the area of coulomb diamonds and coulomb blockade range. The areas of coulomb diamonds are different in Table 1. The spin of tunneling electron is different in each coulomb diamond. The coulomb diamonds of GNR SET with compressive stress of %10Pa on GNR has smaller area than GNR SET with tensile strain of the same amount. Moreover, coulomb blockade range in SET with compressive stress on the island is lower than other counterpart device. Therefore, the performance of GNR SET with compressive stress on the island should be better than GNR SET with the tensile strain of the same amount. This is exactly in agreement with Fig. 3 where the current of the device with compressive stress on its island was higher than the same device with the tensile strain of the same amount.

CONCLUSION

The graphene nanoribbon (GNR) with compressive stress or tensile strain was selected for the island of a single electron transistor (SET). The compact current model of this device was derived incorporating the impact of stress and strain. The impacts of some parameters on the proposed mathematical model was examined. Changing of compressive stress from -3% to -10% and tensile strain from 10% to 3% increased the SET current. Decreasing the numbers of atoms along the GNR length are increased the current due to shortening of the island which was acting as a quantum well. Increasing of the applied gate voltage are raised the current. Moreover, charge stability diagrams for two cases of compressive stress and tensile strain were extracted and compared together. The coulomb diamonds of GNR SET with compressive stress of %10Pa on its GNR island are shown smaller coulomb diamond area and zero current range than GNR SET with the same amount of tensile strain on its island. Because GNR with compressive stress has lower band gap value and then speed of transfer electron is higher than GNR with tensile stress.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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