Uniaxial and torsional strain engineering in Schottky barrier and tunneling CNTFETs

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Abstract: The effects of both uniaxial and torsional strain on the performance of Schottky barrier carbon nanotubes field-effect transistor (SB-CNTFET) and tunneling carbon nanotubes field-effect transistor (T-CNTFET) are examined. This is done by solving the Poisson equation and the Schrodinger equation using the non-equilibrium Green's function (NEGF) formalism under the mode space approach for reduction of computational time. We found that applying the uniaxial or torsional strain can dramatically minimizes the minimum-leakage current, makes the subthreshold swing steeper, and decreases the power delay product (PDP). Switching behavior represented by delay time and cutoff frequency are also studied under strain and we found that compressive strain can enhance cutoff frequency. Such improvement of the device performance can be understood qualitatively to be caused by the band gap modulation in the CNT channel region.
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Key words: strain engineering, carbon nanotubes (CNTs), Schottky barrier, nanoscale transistor, NEGF, PDP.

1. Introduction:

As carbon nanotubes are of great importance, studying strain effects on their properties is becoming an important research topic. Conductance variation of CNT has been proved [1-4] and studied in detail by numerical simulation [5]. Two types of strain can be applied to CNT: uniaxial and torsional strain [6-7]. Both effects have been studied within the range of < 2% [8-9]. In this paper, the change of characteristics of ballistic carbon nanotubes, either Schottky barrier and tunneling FET are studied under both uniaxial and torsional strain. The range of strain is extended to include values ranging from -5% to 7.5% for uniaxial strain. We begin by the calculation of the bandgap of CNT under the effect of strain using [10, eq12]. The change in the hopping parameter is calculated based on Harisson method [11] as:

$$t_j = t_{in}\left(r_{in}/r_j\right)^2 \quad (1)$$

where subscript j= 1, 2, and 3 is the three nearest neighborhoods, t_{in}= 3 eV is a binding parameter between carbon atoms of the unstrained CNT; while t_j is binding parameter after deformation, r_{in} is the length between carbon atoms before strain; and r_j is a bonding length between carbon atoms after strain. Poisson's ratio is considered for the realistic calculation of uniaxial strain and its effect on r_{in}. The Poisson's ratio is defined as the ratio of the circumferential strain to the longitudinal strain with negative sign, i.e.,

$$\nu = \frac{\Delta r/r}{\Delta \ell/\ell} = \frac{\varepsilon_c}{\varepsilon_t} \quad (2)$$

Where r and Δr are initial radius and its change, ℓ and $\Delta\ell$ are lengths before and after strain, ε_c is the circumferential strain, and ε_t is the axial strain [11]. $\nu = 0.2$ is used [12].

We found that the uniaxial or torsional strain has a large effect on the device characteristics such as the ON current, the minimum leakage current, the intrinsic delay, power-delay product *(PDP)* and subthreshold swing *(SS)* due to the variation of the band gap.

2. Approach:

Structures of a T-CNTFET and SB-CNTFET are shown in Fig. 1. In our simulation, we take as example gate all around SBFET. The device has HFO2 as gate insulator of thickness 4nm and dielectric constant of 16. Simulation is performed at room temperature. The channel length is of 20nm and (10, 0) and (19, 0) are used. We studied both axial and torsional strain with a voltage of 0.4 V.

The dc characteristics of ballistic CNTFETs are obtained by the self consistent solution of Schrödinger equation and Poisson equation using the non-equilibrium Green's function (NEGF) formalism under the mode space approach for reduction of computational time. A tight-binding (TB) model is included in the Hamiltonian with a p_z orbital basis set. We extended our previous work [13-14] to include the effect of uniaxial or torsional strain by calculating the band gap of the CNTs in case of uniaxial or torsional strain using [10, eq.(12)]. Then, we introduced the uniaxial strain in the NEGF formalism by the same method presented in ref. [9].

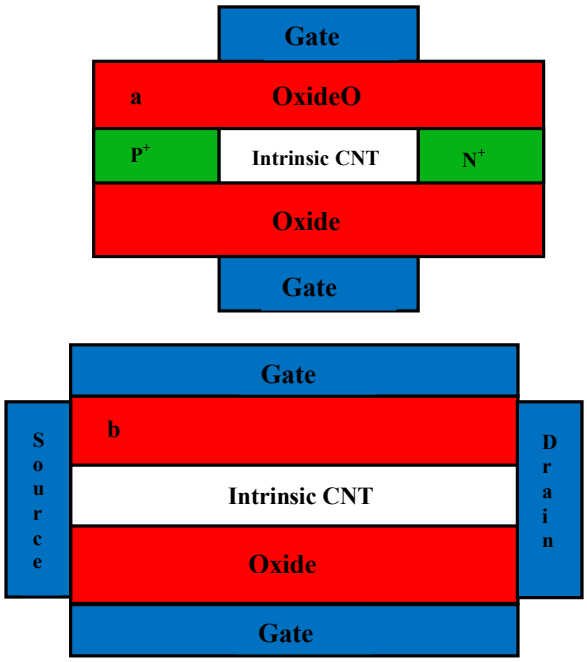


Fig. 1 Cross section of the a) T-CNTFET and b) SB-CNTFET.

3. Results:

A. Band gap versus uniaxial or torsional strain

The band gap change of the CNTs due to uniaxial or torsional strain is found from [10, eq. (12)].Figure 2 shows the band gap modification of (10, 0) and (19, 0) under uniaxial strains. The inset figure illustrates the band gap variation by torsional strains.

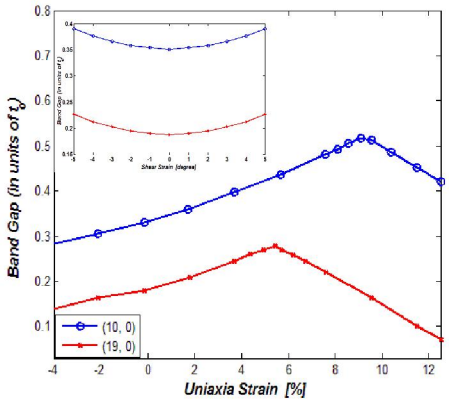


Fig. 2 Energy gap variation under different uniaxial strain. The inset figure shows the energy gap variation with torsional strain

We found that under uniaxial strain, the variation of the energy gap with strain is independent of diameter and can be approximated as $3t_0$. In case of torsional strain, it takes a small value. It must be noted that there is an abrupt reversal in sign of $dEg/d\sigma$ in zigzag tube for high values of stain. The point at which reversal of sign occur depends on the diameter [10]. For example, for the (19, 0) tube, the change in slope occurs at around five percent strain while for (10, 0) tube the change in slope occurs at around nine percent strain.

B. I_{DS}–V_{GS} Characteristics

The most important performance parameter to be studied is the drain current. **Error! Reference source not found.** plots I_{DS}-V_{GS} characteristics with different uniaxial strain effect on (a) a SB-CNTFET with (10, 0) CNT and (b) a T-CNTFET with (19, 0) CNT channel, and. From the figure, it is clear the large change of current with strain. The change of current with uniaxial strain for (10, 0) can be explained as follows. From Fig.2, it is found that the band gap increases with strain. We obtain a higher SB and thus current decrease. For compressive strain, the band gap decreases and SB height is decreased and current is increased.

Error! Reference source not found. plots I_{DS}-V_{GS} characteristics with different torsional strain on (a) a SB-CNTFET with (10, 0) CNT and (b) a T-CNTFET with (19, 0) CNT channel. The reduction of drain current with torsional strain is expected from band gap variation with shear strain as shown in the inset of **Error! Reference source not found.**. The increase of shear results in the increase of the energy gap with in its turn increase the SB height and reduces the current. It is found that the torsional strain is dependent only on the angle value and not on its direction. The change of current due to strain is important even for small values of strain. Starting with values of 1% results in current change, that is clear from Fig.4.

Because SB-CNTFETs and T-CNTFETs show ambipolar I–V characteristics, leakage current increases. The OFF current is strongly dependent on the minimal leakage current and strongly affects device performance. From Fig.3 and Fig. 4, it is clear that I_{min} is reduced by applying strain resulting in enhancement in device performance. The leakage current is decreased approximately by 2 orders of magnitude as the strain is increased by 2% for SB-CNTFET. The same effect of I_{min} decrease is found for T-CNFET but with smaller rate.

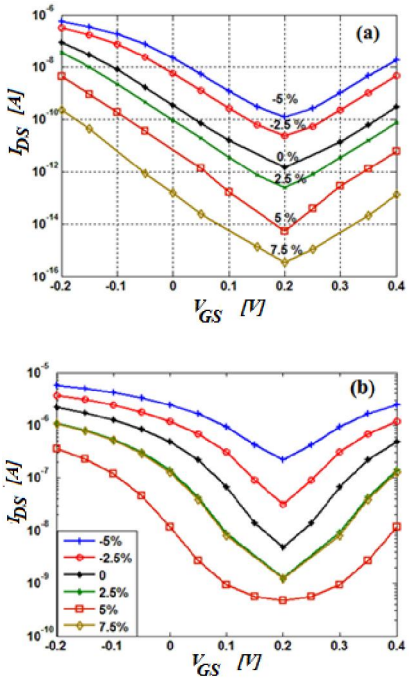
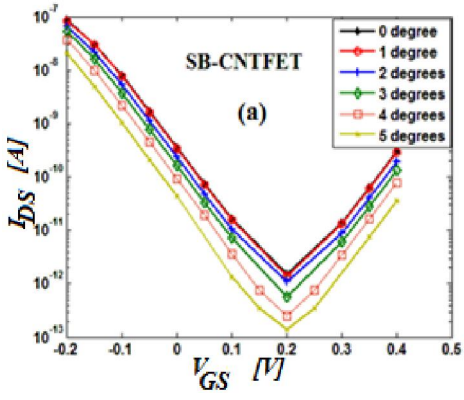


Fig. 3 I_{DS}-V_{GS} characteristics for several uniaxial strain values of a) SB-CNTFET and b) T-CNTFET



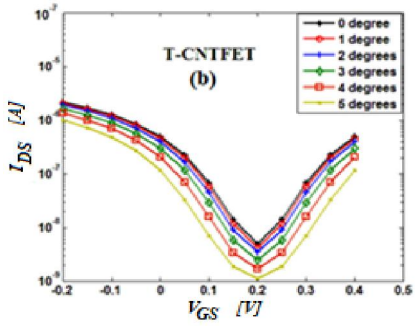


Fig. 4 I_{DS} versus V_{GS} for several torsional strain values for a) SB-CNTFET and b) T-CNTFET.

C. Subthreshold Swing(SS)

The subthreshold swing is an important parameter in transistor performance. Low power operation of transistor allows its scaling to small sizes [15]. Fig.5 shows the subthreshold swing (SS) under different values of the uniaxial strain as a function of V_{GS} for the studied structures. The 60 mV/dec limits also shown. According to the subthreshold swing definition [15], for a given V_{GS}, it calculates as follows:

$$SS = 10^3 \frac{V_{GS2} - V_{GS1}}{\log(I_{DS2}) - \log(I_{DS2})} \left(mV/dec\right) \quad (3)$$

Where V_{GS2}, I_{DS2} and V_{GS1} and I_{DS1} are gate-source voltage and drain current. *SS* indicates to the subthreshold swing. As seen from Fig.5, in both structures, the subthreshold swing is sharper in case of uniaxial strain. The application of strain does not change the behavior of SB-CNFET, the subthreshold swing is still larger than 60mV/dec.

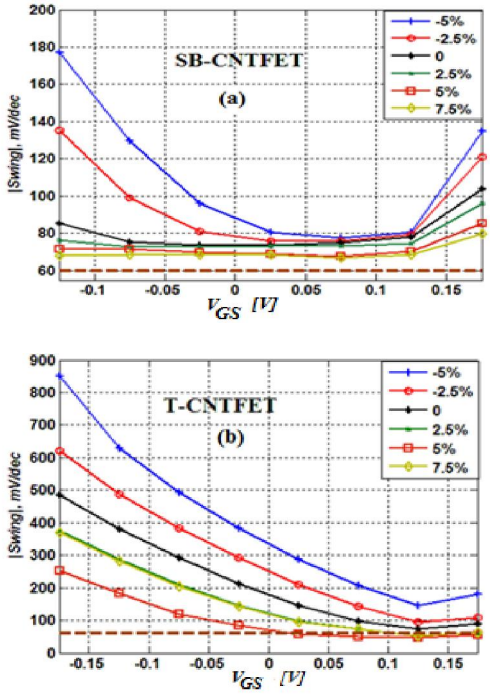


Fig. 5 Plot of the subthreshold swing versus V_{GS} for the (a) SB-CNTFET and (b) T-CNTFET, for various values of the uniaxial strain.

D. Switching behaviors

Now, we want to explore the effect of uniaxial strain on switching behaviors. The most important parameter in the switching behaviors of transistor is the delay time, defined by:

$$\tau = \frac{(Q_{ON} - Q_{OFF})}{I_{ON}} \quad (4)$$

It indicates the speed of transistor switching. We can also define another important parameter for switching parameter, the power-delay product (*PDP*) that is defined as:

$$PDP = (Q_{ON} - Q_{OFF})V_{DS} \quad (5)$$

It related with the energy efficiency of a logic gate. Known as switching energy, PDP, is the product of the power consumption and the delay time. It has the dimension of energy and measures the energy consumed in each switching. [16]. $Q_{ON/OFF}$ is the total charge during the ON/OFF state. We evaluated delay time and *PDP* versus uniaxial strain as shown in Fig. (6-a) and Fig.(6-b) respectively. The effect of uniaxial strain has an increasing effect on the delay time while a decreasing the PDP. Then, uniaxial strain enhances can power consumption but not all other performance metrics.

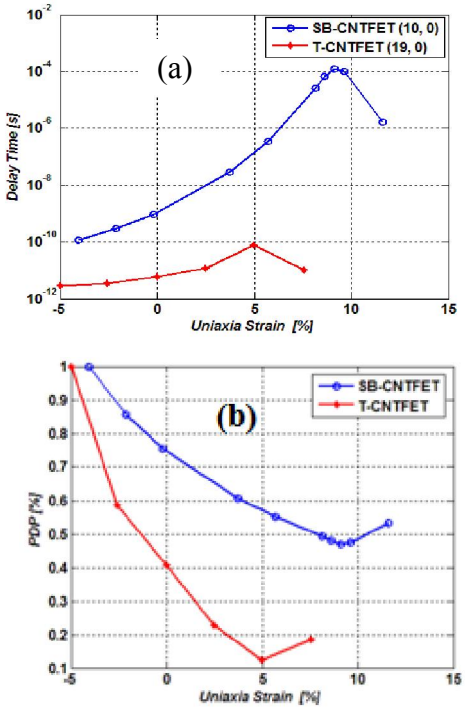


Fig. 6 (a) Delay time and (b) PDP, versus uniaxial strain

E. Cutoff frequency

The cutoff frequency is a very important parameter that determines the range of operation of the device. It is calculated as:

$$f_T = \frac{1}{2\pi}\frac{g_m}{C_g} \quad (6)$$

Where C_g is the total gate capacitance including gate oxide capacitance, quantum capacitance and capacitance that correspond to field terminating on source and drain regions [17,18].

$$C_g = \frac{\partial Q_g}{\partial V_g} \quad (7)$$

The total gate charge for a tube of radius R and channel length L_g and relative permittivity ε_r is found from the following equation:

$$Q_g = 2\pi R \int_{Lg} \varepsilon_o \varepsilon_r E(x) \quad (8)$$

Moreover, g_m is the transistor transconductance defined as

$$g_m = \frac{\partial I_D}{\partial V_{GS}} \quad (9)$$

The results shown in Fig.7, show that the uniaxial strains enhance the cutoff frequency in case of compressive strain.

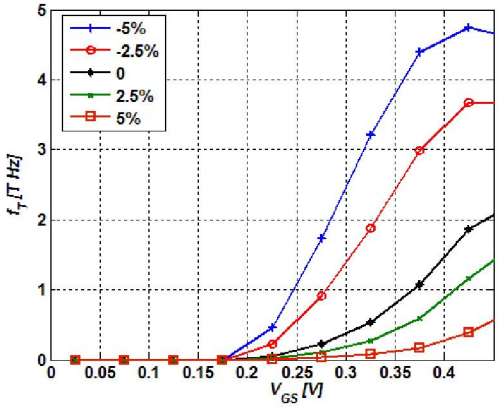


Fig.7: Cutoff frequency f_T versus gate bias under different uniaxial strain.

4. Conclusion:

Band gap variation of CNT is generated with uniaxial and torsional strain and is investigated using NEGF formalism. To generalize our work, we have considered two different types of semiconducting zigzag CNTs, (10, 0) and (19, 0). The effects of uniaxial and torsional strain on the characteristics of the ballistic SB-CNTFETs and T-CNTFETs are studied. We found that applying the uniaxial or torsional strain can dramatically minimizes the minimum-leakage

current, makes the subthreshold swing steeper, and decreases the power delay product (PDP). Such enhancement of the device performance is explained qualitatively to be caused by the band gap variation in the CNT channel region. The cutoff frequency, which is a critical parameter in transistor behavior, has also been studied. The results show that compressive strain can largely enhance f_T.

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