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Improving I_{on}/I_{off} in dual-gate graphene nanoribbon field-effect transistors using local uniaxial tensile strain



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HIGHLIGHTS

• We present the Dual-Gate Graphene Nano Ribbon Field Effect Transistor (DG-GNRFET) under local uniaxial strain in source and drain regions.

- We examine the changes in the level of strain's strength, position and length to find the optimum performance of device.
- We compare the results to a conventional device.
- We report a high Ion/Ioff ratio besides a high on-current.
- We show that short channel effects should be better in the proposed device.

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1. Introduction

Graphene, as a single-layer hexagonal lattice of carbon atoms with extraordinary physical properties, after its invention by Novoselov [1] has attracted a great deal of attention. Graphene with its massless π -electrons at Dirac points near Fermi energy provides a two-dimensional electronic platform [2–4] with high electron mobility [5], super thermal conductivity [6], no backscattering and Klein tunneling [7]. However, graphene's zero energy gap is the major drawback that limits its usage in some applications.

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ABSTRACT

In this work, we present the Dual-Gate Graphene Nano Ribbon Field Effect Transistor (DG-GNRFET) under local uniaxial strain in source and drain regions as a device suitable for switching applications. Our investigations are based on the 2D Poisson based on an atomistic mode-space approach and Schrodinger equations, within the Non-Equilibrium Green's (NEGF). We show a high on-current and on-off ratio which can be obtained using the combination of techniques such as applying uniaxial strain to the portion of channel/source regions and the gate overlap. We followed an optimization process to find the best performance of the device. Finally, the proposed device shows a higher on-current and on-off ratio becomes about 100 times greater than of the unstrained device.

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Nonetheless, armchair graphene nanoribbons (A-GNRs) of widths 10 nm or less become semiconductors and have an energy band gap which is suitable for transistor channels [8,9]. As mentioned in the literature, all AGNRs are semiconducting with bandgaps well separated into three different groups n=3p, n=3p+1; n=3p+2. However, the bandgap of the family n=3p+2 is significantly reduced resulting in a close-to-metallic channel. On the other hand, the groups n=3p and n=3p+1 have larger bandgaps and are more promising for FET applications. Recent studies show that AGNRs with n=3p is more better from the on-current point of view and have higher maximum cutoff frequencies obtained at lower gate biases and hence, are preferable for high frequency applications. But the family n=3p+1 seems to be most suitable for switching applications [10]. Regardless of the family type,



recent studies reveal that strain has great impacts on the mechanical, optical and electronic properties of graphene and AGNRs [11–17]. It has been experimentally shown that graphene is strong enough to bear strains up to 30% [12]. It has also been experimentally proven that local strains rather than being introduced directly into graphene can be introduced indirectly by devising patterns such as trenches, dots, or wells into the substrate or the oxide layer beneath the graphene sheet [12,13]. Moreover, it has been demonstrated that introduction of uniaxial strain can modulate A-GNRs band gaps in a periodic manner, whose details strongly depend on the GNR width [14]. Taking advantage of these can be beneficial to the use of strain in the channels of GNR-FETs [15–20].

In our most recent study, we have demonstrated that when 5% uniaxial strain is uniformly applied across the channel of a dual gated GNR-FET consisting a 10-nm long (12, 0) A-GNR, I_{on}/I_{off} ratios of higher than 10⁶, and also sub-threshold slopes as low as 13 mV/ dec can be obtained. This slope is much less than 60 mV/dec limit for ordinary MOSFETs [11]. When the strain is applied uniformly across the channel, any uniform variation in it increases/decreases the GNR bandgap, uniformly across the GNRFET channel [11,18– 21]. This would weaken/enhance the band to band tunneling (BTBT) mechanism uniformly and meanwhile the device on-current, decreases/increases. On the other hand, the weakened/enhanced BTBT decreases/increases the off-current ultimately. In other words, varying the uniform uniaxial tensile strain across the GNRFET channel increase/decrease the device on- and off-currents at the same manner. However, as demonstrated in [11], these variations are such that when on-current increases the on/off ratio decrease and vice versa. That is, the amount of increase in offcurrent is more than that in the on-current and vice versa. In order to overcome this deficiency in conventional MOSFETs, one way is to use local uniaxial strain such as used for tunneling FETs [20–22].

In this work, we apply a local strain around the junction of source and the channel of a dual-gate field effect transistor (DG-GNRFET).

In this paper, we developed a new Local Uniaxial strain in Source and Drain dual-gate GNR-FET (LUSD-GNRFET) by applying a locally uniaxial strain in source and drain. Here we investigate its performance by means of numerical simulations which self-consistently solves the 2D Poisson based on an atomistic mode-space approach and Schrodinger equations, within the Non-Equilibrium Green's (NEGF) [11]. Comparison of the conventional GNRFET and the proposed model show that our proposed device have a larger on-current (I_{on}) and ON–OFF ratio (I_{on}/I_{off}) and superior ambipolar characteristics. Simulations show that applying uniaxial strain besides extending gate into the source and drain suppress the BTBT mechanism and minimize the off current without undesirable effect on the ON-current.

The paper is organized as follows. In Section 2 we introduce the proposed device structure and the simulation method. Section 3 contains the simulation results and related discussions. In Section 4, we will conclude the paper.

2. Device structure and simulation approach

Fig. 1 illustrates the 2 dimensional cross sectional view of the proposed GNRFET with a uniaxial strain applied to the portion of source and drain in the presence of gate overlap that we call it as LUDS-GNRFET hereafter. In this structure, the armchair GNR (A-GNR) is sandwiched between two 1.5 nm insulator layers of SiO₂ with ε_r =3.9. The channel is taken to be intrinsic and the heavily doped source and drain regions are assumed to be $5 \times 10^8 \text{ m}^{-1}$ to provide good electrical conduction. The GNR used for simulation is armchair edge and referred to as *n*-GNR. Here, *n* is the number of



Fig. 1. Simulated device schematic showing parameters definition.

dimmer lines across the nanoribbon width and equals to 12. The n=12 GNR belongs to n=3p family which initially has a reasonable band gap. The band gap of this family of GNRs increases by increasing uniaxial strain unlike what occurs in n=3p+1 family. It is well known that this type of GNR is a semiconducting material that is suitable for the device under consideration [11]. The width and length of this GNR channel is assumed to be W=1.35 nm and L=10 nm, respectively. These parameters are chosen to make the unstrained DG-GNRFET comparable to that of simulated in [9,11]. The overall lengths of the source and drain regions are all equal to 30 nm. The gate overlap and the length of the regions of source and drain under strain are defined as L_{ov} and L_{str} respectively. Note that for $L_{ov}=L_{str}=0$, the device shown in Fig. 1 is the same as conventional DG-GNRFET and simulated in [11] for the channel under different uniaxial strains. The effect of strain is modeled by modifying the tight binding parameter based on Harrison's formula, $t_i = t_0 (r_0/r_i)^2$. Here, t_0 , r_0 are the hopping parameter and the carbon-carbon bond length, respectively, of the unstrained GNR, and r_i is the bond length of strained GNR. With the uniaxial strain applied, the x and y components of a carbon-carbon bond are calculated by the following Eq. [8]:

$$\begin{aligned} r_{ix} &= (1 + \varepsilon_x) r_{0x}, \\ r_{iy} &= (1 - \nu \varepsilon_x) r_{0y} \end{aligned} \tag{1}$$

where, ε_i is the uniaxial strain and $\upsilon \approx 0.14$ is the Poisson ratio [23]. The details of constructing effective Hamiltonian of the modeled device under uniaxial strain in mode space are described before [11]. The analytical model for calculating band gap and effective mass versus strain was developed earlier [10,11], [24]. The relation between 12-AGNR and the uniaxial tensile strain was depicted in [11]. To clarify, we illustrates these common zigzag variations for n=9 to n=18 AGNRs in Fig. 2, similar to those reported by [11,15]. As it is seen, E_g in the range of tensile strain 0% $\leq \varepsilon \leq 15\%$ increases first and then decreases linearly. Therefore there is a turning point, i.e., as the strain increases, there is an abrupt reversal in the sign of $dE_g/d\epsilon$, making the curves to display a Λ shape. The turning point moves towards smaller values of strain as the width of AGNR increases. The above observations is in agreement with the variation of effective mass at the conduction band with ε [24]. As it is clearly seen in Fig. 2(b), m^* has similar strain dependence as E_{g} and a linear between m^{*} and E_{g} is expected which could be correlated to an inverse relationship between mobility and band gap. As shown in Fig. 2(b), the initial band gap value is 0.8168 eV and increases to 1.243 eV when the strain strength grows up to 5% and reduces for ε beyond 5%.

In order to better understand, we compare our results with those reported in [11] with doping concentration of 5×10^8 m⁻¹ in S/D regions ($N_{\rm SD}$). In order to find the optimum length and strength of strain, we start changing each of the parameters such as length of strained region, strain strength and gate overlap individually.

The device characteristics are simulated by solving the ballistic

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