Achieving a higher performance in bilayer graphene FET – Strain Engineering

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Abstract—**In addition to its high mobility, the possibility of opening sizable bandgaps has made bilayer graphene (BLG) a promising candidate for many electronic and optoelectronic applications. Yet, the achievable bandgap (300 meV) is not sufficient to make BLG a candidate for high performance transistors. Vertical strain in conjunction with the vertical field can help to achieve a larger band gap in BLG. In this paper, p_z nearest-neighbor atomistic tight-binding model and Non-equilibrium Green's Function (NEGF) method are used to study the transport behavior of strained BLG transistors under electric field. A field tunable dynamic band gap (DBG) of up to 300 meV is found to exist in BLG with no strain in agreement with previous reports. By applying strain, one can increase the band gap of BLG beyond 300 meV. Finally, the DBG effect and vertical strain are shown to be able to enhance the ON/OFF ratio of a BLG field effect transistor (FET) to 1000.**

Keywords—Bilayer Graphene, Field Effect Transistor, Dynamic Bandgap, Strain

I. INTRODUCTION

Two-dimensional materials have been shown to be good candidates for future low power electronics [1-4]. In this regard, graphene has attracted great interest due to its extraordinary physical, chemical, and electrical properties. Its many unique features including a high carrier mobility, easy fabrication and lithography make it a promising candidate for next generation transistors [1]. However, due to the lack of an intrinsic band gap, graphene transistors cannot be turned off. To overcome the zero band gap problem, several methods have been developed so far: 1) applying a vertical electric field to bilayer graphene (BLG) [5], 2) inducing strain on graphene [6].

As predicted by the International Technology Roadmap for Semiconductors, silicon field effect transistors (FETs) will reach its physical limits in 1-to-2 decades due to short channel effects [7]. Graphene FETs need an energy band gap of at least 400 meV to be a promising alternative of Si [8]. Both theoretical, and experimental results show that the maximum achievable energy gap induced by electric field in BLG is about 300 meV. On the other hand, strain has also been demonstrated as a technique to open up a band gap in graphene [9]. Here, the transport properties and performance of BLG FETs under application of both strain and electric field are investigated using atomistic simulations.

This report first evaluates the bandgap of the BLG from tight-binding calculations. A bandgap of 300 meV can be created employing a vertical displacement field of 6V/nm in this zero bandgap semiconductor. A BLG transistor with a top and a bottom gate with opposite biases is considered here to exploit this tunable bandgap behavior. The electric field is created through the voltage difference of these two gates. The transmission of this transistor is shown to follow the corresponding electric-field dependent band structure. This verifies that the DBG behavior is captured in the transport model.

To include the strain effect in atomistic simulation, Boykin's model is used [10]. It is shown that strain further increases the band gap of BLG in addition to the vertical field. The saturation band gap value increases with an increasing vertical strain. Thus, the ON/OFF ratio also increases with a vertical strain.

The simulation results reveal the following facts about performance of BLG FETs in room temperature: 1) an ON/OFF ratio of 100 can be achieved in the double gated BLG FETs without strain and 2) a vertical strain of 9% can increase this ON/OFF ratio to 1000.

II. METHOD

Here, the AB (Bernal) stacking BLG Hamiltonian is constructed based on the p_z nearest-neighbor atomistic tight-binding model. Perpendicular strain ε, associated with a change from the interlayer distance c to $c' = c(1+\varepsilon)$ is also included. Here c equals *0.335*nm. The whole Hamiltonian including vertical strain can be expressed as [10]:

$$H = \begin{bmatrix} +V + c\frac{\partial V}{\partial c}\varepsilon & \hbar v_F k e^{i\phi(k)} & t_\perp + c\frac{\partial t_\perp}{\partial c}\varepsilon & 0 \\ \hbar v_F k e^{-i\phi(k)} & +V & 0 & 0 \\ t_\perp + c\frac{\partial t_\perp}{\partial c}\varepsilon & 0 & -V + c\frac{\partial V}{\partial c}\varepsilon & \hbar v_F k e^{-i\phi(k)} \\ 0 & 0 & \hbar v_F k e^{i\phi(k)} & -V \end{bmatrix} \quad (1)$$

The variation of hopping parameter $t_\perp$ with interlayer distance c, $\frac{\partial t_\perp}{\partial c}$ is estimated using Boykin's model [11]. v_F is

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the Fermi velocity of graphene, $1 \times 10^6 m/s$. $\frac{\partial V}{\partial c}$ is evaluated in Ref. 10. $\phi(k)$ equals $\frac{\pi}{6}$ at Dirac point.

Bilayer graphene FETs have been simulated using the self-consistent Poisson-Non-Equilibrium Green's Function (NEGF) method through our Nano-Electronic MOdeling (NEMO5) tool [13-15]. The material properties are listed in Table I.

Table I: Bilayer graphene material properties: maximum field induced bandgap *Eg*, electron effective mass m_e*, in-plane and out-plane relative dielectric constant ϵ_r^{in} and ϵ_r^{out}. *Eg* and m_e* are obtained from the bandstructure calculations while ϵ_r^{in} and ϵ_r^{out} are input parameters to the Poisson equation.

Parameters	*Eg (meV)*	m_e* (m_0)	ϵ_r^{in}	ϵ_r^{out}
BLG	275	0.038	3	3.3

III. Results

Fig. 1 shows how the band structure of BLG changes with a vertical electric field applied between the two graphene layers. The bandgap increases linearly with the small electric fields and saturates at 300meV for high electric fields. Notice that the band edge without electric field is at K point. However, band edges moves away from K-point by increasing the field.

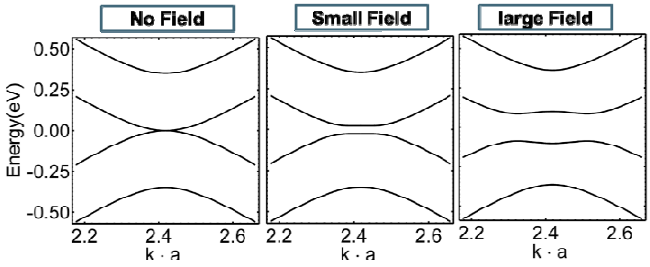

FIG. 1. Bandgap of bilayer graphene changing with a vertical electric field. The bandgap increases with an increasing field up to a saturation point.

Fig. 2 presents the bandgap as a function of the displacement field. The bandgap of BLG can be adjusted from zero up to 300meV and saturates at a displacement field of 6V/nm.

The average displacement field in simulation and experiment are calculated differently. In the simulation, the effect of electric field is calculated by setting constants $+V$ and $-V$ as the onsite energies of the top and bottom layer atoms. Average vertical displacement field, D_{av}, then equals $2V/c$. Experimentally, the average displacement field of top and bottom gates are considered:

$$D_{av} = \frac{1}{2}[\epsilon_{top\_ox} \cdot \frac{V_{TG}}{t_{top\_ox}} - \epsilon_{bot\_ox} \cdot \frac{V_{BG}}{t_{bot\_ox}}].$$

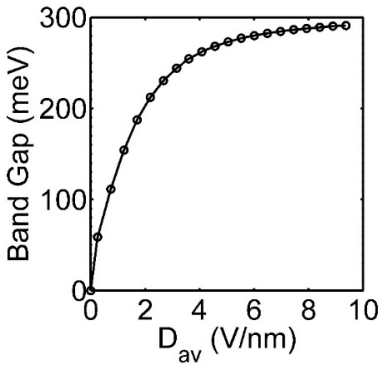

FIG. 2. Dynamic bandgap (DBG) in BLG as a function of the displacement field.

Fig. 3 shows the transmission results from NEGF and the corresponding band structures. Two scenarios are presented: 1) Without an electric field, the transmission through the zero bandgap BLG is finite. 2) In contrast, a bandgap opens up with an electric field of 1V/nm and results in zero transmission through the bandgap. This verifies the formation of a transport gap besides the optical gap in BLG under vertical field.

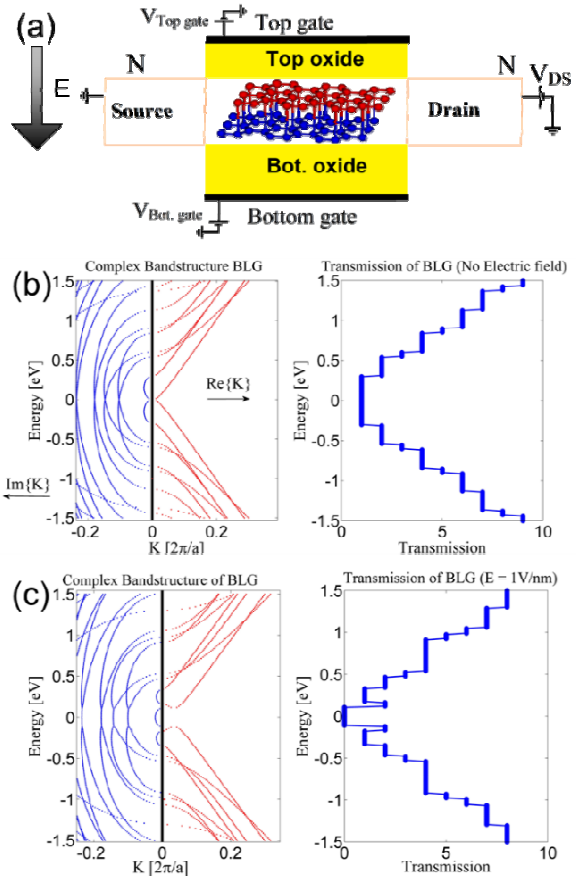

FIG. 3. (a): Bilayer graphene FET device and atomic structure. Bandgap and transmission for a BLG device in a small (b) and large (c) electric field.

If not stated otherwise, all the simulation results discussed are for a double gated bilayer graphene structure shown in Fig. 4.

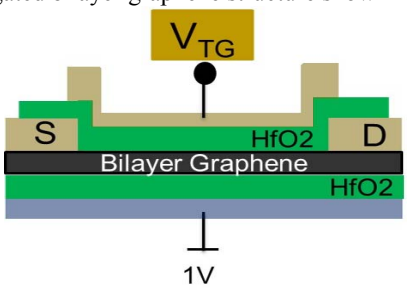

FIG. 4. Schematic of the double gated bilayer graphene field effect transistor used in this work.

Fig. 5 shows the transfer characteristics of BLG FET at temperature of 300 K obtained from Poisson-Non-equilibrium Green's Function (NEGF) method. V_{DS} is 10mV, and the Fermi level is fixed to 0eV. The back gate voltage V_{BG} is set to 2V. Despite the band gap increasing with the top gate voltage (V_{TG}), the device is ON, then OFF, and ON again (marked as 1, 2 and 3 respectively) with the sweeping of top gate and generates a **V** shaped I-V characteristic.

From the potential energy at top and bottom graphene layers, extracted from self-consistent simulations, one can calculate the conduction and valence band edges which are called "local band structure" here. "Local band structure" is plotted in Fig. 5 by extracting the band edges for each unit cell. Not only does an increase in the top gate bias pull down the band edges in the channel, but it also increases the bandgap. Despite this monotonic increase in the bandgap, the OFF state occurs when the middle of the bandgap aligns with the Fermi level (shown as (2) in Fig. 5). Further increase in VTG and consequently the band gap does not decrease the current since the band gap is not blocking the thermal window (shown as (3) in Fig. 5).

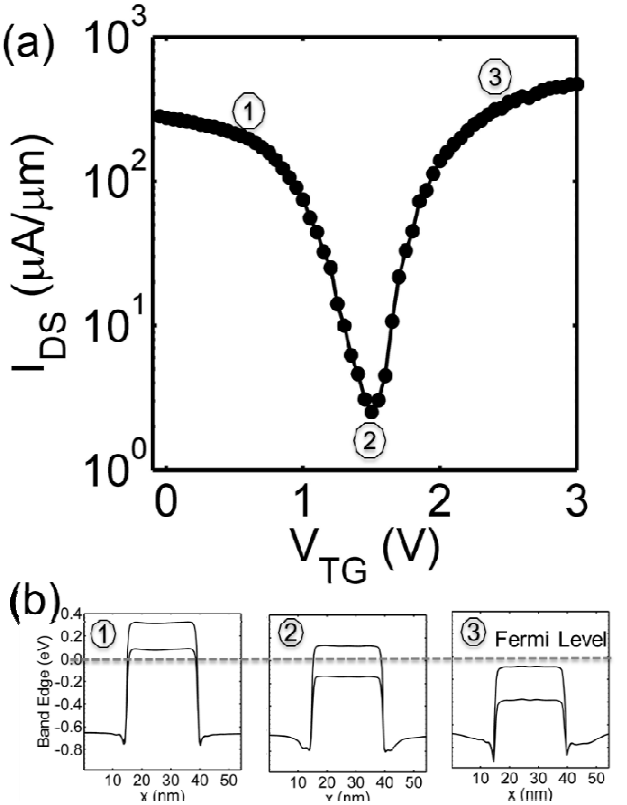

FIG. 5. (a): **V** shaped transfer characteristics of bilayer graphene double gate FET. (b): band edge plot along transport direction for the ON, OFF and ON state.

In the Hamiltonian matrix exhibited by (1), the change of onsite energy of different layers due to vertical electric field is presented by the constant +V and –V. In the four atom unit cell, vertical strain ε breaks the symmetry of the two atoms within a layer since only one of these two atoms is connected to the other layer. Interestingly, the Hamiltonian (1) displays a possibility of opening a strain induced band gap. Verberck et al. examined this possibility and found out that in specific conditions strain by itself can open a band gap: $\left|c\frac{\partial V}{\partial c}\varepsilon\right| > t_\perp + c\frac{\partial t_\perp}{\partial c}\varepsilon$ [10].

As shown in Fig. 6, strain has two major impacts on the band structure of BLG. 1) Producing asymmetric conduction and valence bands. This is due to the fact that in the presence of vertical strain, the onsite energies of the in-plane carbon atoms in each layer of graphene become asymmetric. 2) Creating a larger band gap in the presence of a vertical electric field. Electric field here is evaluated using the inter plane distance c' after straining.

Based on the band structure calculations, one can open a larger band gap by pulling apart the two layers of graphene in the existence of vertical electric field. Similar conclusion can also be found in Ref. 10.

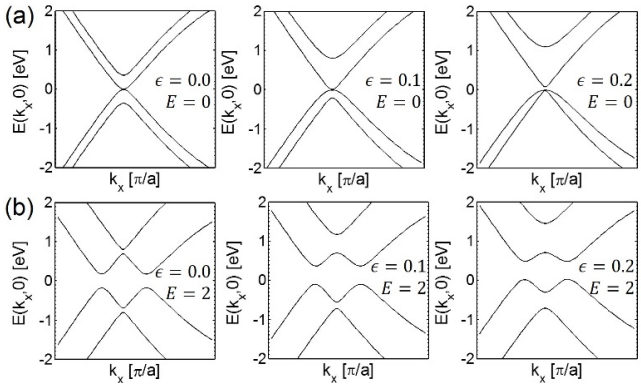

Fig. 6 Band structure of strained bilayer graphene without (a) and with (b) vertical field [V/nm]. Left, middle and right figures correspond to band structures of bilayer graphene with different strain values.

The effect of strain and vertical field are demonstrated in Fig. 7 more clearly. Fig. 7a shows that the application of strain can increase the band gap when the vertical field is higher than 0.4V/nm. Moreover, the impact of strain is more significant in the higher vertical field values. Fig. 7b shows the band gap as a function of vertical field for different strain values; higher the strain, larger the maximum value of the band gap. This effect indicates that with a vertical strain, it is possible to achieve a higher ON/OFF ratio in bilayer graphene transistors.

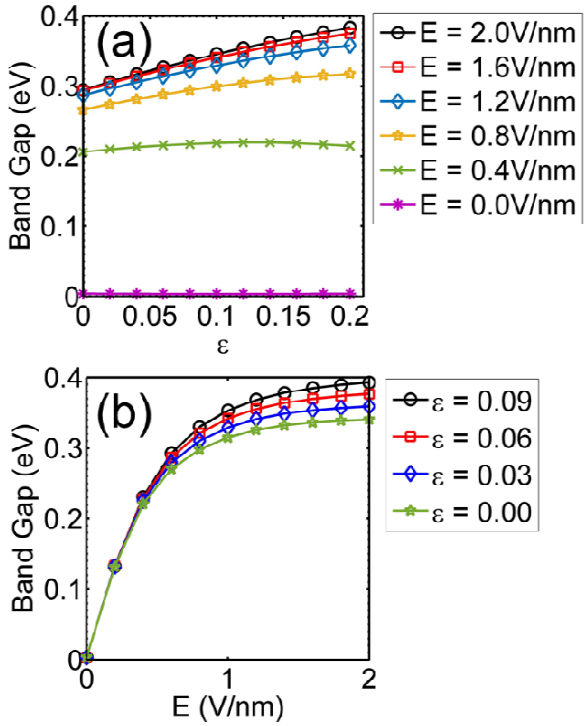

Fig. 7 (a) Band gap changes with strain applied in different vertical fields [V/nm]. (b) Band gap increases with vertical field. Saturation band gap increases with larger strain.

Fig. 8 shows the transfer characteristics of a double gated bilayer graphene transistor. The devices with higher applied strain can achieve a higher ON/OFF ratio. A 9% strain leads to ON/OFF ratio of 10^3, compared to 10^2 without strain. Notice that the strain mainly reduces the OFF current and keeps ON current intact since the strain impacts the band gap.

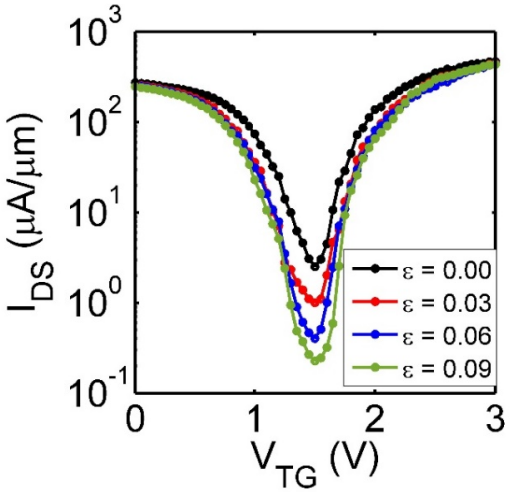

Fig. 8 IV curves for double gate bilayer graphene devices applied with different vertical strain.

IV. Conclusion

In conclusion, vertical electric field combined with vertical strain can achieve a larger bandgap in bilayer graphene, compared to the unstrained case. The increase in band gap helps double gate BLG devices to achieve a higher ON/OFF ratio.

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