Intrinsic limits of subthreshold slope in biased bilayer graphene transistor

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(Received 12 February 2010; accepted 23 February 2010; published online 23 March 2010)

In this work, we investigate the intrinsic limits of subthreshold slope in a dual gated bilayer graphene transistor using a coupled self-consistent Poisson-bandstructure solver. We benchmark the solver by matching the bias dependent band gap results obtained from the solver against published experimental data. We show that the intrinsic bias dependence of the electronic structure and the self-consistent electrostatics limit the subthreshold slope obtained in such a transistor well above the Boltzmann limit of 60 mV/decade at room temperature, but much below the results experimentally shown till date, indicating room for technological improvement of bilayer graphene. © *2010 American Institute of Physics*. [doi:10.1063/1.3364142]

The excellent transport properties of single and multilayer graphene hold promise to build ultrafast transistors with excellent on state characteristics.[1–4] However, the lack of significant band gap in such systems has been one of the major roadblocks to achieve low off state current and hence high on/off current ratio.[2–4] Recently, it has been found, both theoretically and experimentally, that a band gap can be opened up in a bilayer graphene (BLG) using an external bias.[4–10] A recent experiment shows that a band gap as large as ~0.3 eV can be created in a BLG depending on the external bias.[6] This relatively large band gap is promising to obtain low off state current, hence an improved on to off current ratio and subthreshold slope.[10]

The aim of this paper is to discuss the intrinsic limits of the subthreshold slope in a BLG metal-oxide-semiconductor field effect transistor (MOSFET). We assume a long channel transistor with an ideal gate dielectric interface. To achieve this, we develop a self-consistent Poisson-bandstructure solver for a dual gated BLG device. We have simulated the magnitude of the bias dependent band gap tuning in a BLG system which matches closely with the published experimental data[6] validating the solver. We also show that the gate bias dependent electronic structure and the self-consistent electrostatics play a central role in determining the intrinsic limits of the subthreshold slope in a BLG transistor, which remains well above the Boltzmann limit of 60 mV/decade.

A schematic of the BLG device configuration is shown in Fig. 1(a) where a BLG is sandwiched between a top and a bottom gate stack. Each gate stack consists of a gate dielectric with an equivalent oxide thickness of 1 nm and a gate contact metal. We assume perfect dielectric-BLG interface and zero flatband voltage. The voltage at the top gate (V_t) and the bottom gate (V_b) can be varied independently. The self-consistent electronic structure of this device configuration is determined by the bandstructure of the BLG using tight binding method[1,9] coupled with the one-dimensional Poisson equation. Taking the center of the two graphene layers at $z=0$, the charge density is given by $\rho(z)=qn(z)$ where q is the electronic charge and $n(z)$ is the difference between the hole $[n_h(z)]$ and electron $[n_e(z)]$ carrier density,

$$n(z)=2\left(\sum_{i,\bar{k}}\{1-f[E_i(\bar{k})]\}|\psi_i^{\bar{k}}(z)|^2-\sum_{j,\bar{k}}f[E_j(\bar{k})]|\psi_j^{\bar{k}}(z)|^2\right), \quad (1)$$

where $f[E_{i,j}(k)]$ is the Fermi–Dirac probability of the state $(\{i,j\},\bar{k})$ at temperature T. i and j are the valence and conduction band indices respectively. The energy eigenvalues $E_{i,j}(\bar{k})$ are obtained from the tight binding bandstructure taking only p_z orbital into account, with an intralayer overlap integral (S) of 0.129, the intralayer hopping t as -3.033 eV and interlayer hopping $t_\perp$ as -0.365 eV.[1] To obtain the wave function $\psi_i^{\bar{k}}(z)$, we assume normalized Gaussian orbital as the basis function.

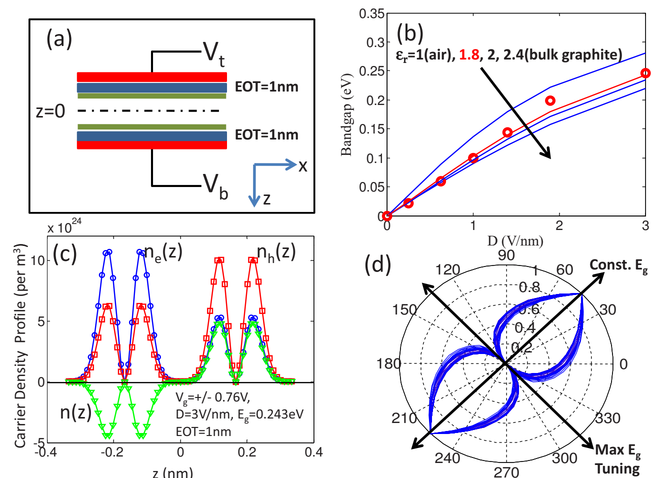

FIG. 1. (Color online) (a) Schematic of a bilayer graphene (BLG) sandwiched between two gate stacks. (b) Verification of numerically obtained band gap results with experimental data in Ref. 6, shown as circles. (c) Carrier density profiles from top layer to bottom layer. (d) Polar plot of the rate of change of B_e (normalized by q) along different directions using Eq. (2) [with angle $\theta=\tan^{-1}(V_t/V_b)$] in the (V_t,V_b) space for two sets of subthreshold points: (i) $V_t=-1$ V, $V_b\in[0V,1V]$ and (ii) $V_t=-0.5$ V, $V_b\in[0V,0.5V]$. All the curves show similar directional dependence.

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We validate the above method by setting V_t to $-V_b$ to break the inversion symmetry[4,5] and comparing the bias dependent bandgap results with Ref. 6. The results are shown in Fig. 1(b) where the band gap (E_g) is plotted as a function of the average displacement vector D, defined in the same way as in.[6] Here the relative permittivity (ϵ_r) of BLG is varied as a parameter to find that $\epsilon_r=1.8$ provides the best fit to the experimental data and the same value is used in the rest of the paper. Figure 1(c) shows the carrier density profiles along z at $D=3$ V/nm. This clearly shows a strong charge polarization in the bilayer, though the system as a whole remains almost neutral for $V_t=-V_b$.

The recent development of significant tunability of band gap in a bilayer graphene[5–10] brings the possibility of significant reduction of off current in a BLG transistor. In the following, we show that the bias dependent electronic structure and the corresponding self-consistent electrostatics play a major role in determining the intrinsic limits of the subthreshold slopes and the on/off current ratio in an ideal long channel BLG MOSFET.

Before discussing the self-consistent results, we first show that even in absence of the screening effect, the intrinsic bias dependence of the electronic structure in BLG can be a major cause for subthreshold slope degradation. This arises from the dependence of the rate of change of electron and hole barrier height ($B_{e,h}$) with gate bias. This rate, ideally, should be as high as possible, with the maximum possible value being 1, which corresponds to a subthreshold slope of 60 mV/decade at room temperature. This is obtained by finding the roots λ of the secular equation of the bilayer Hamiltonian matrix (with $S=0$),

$$[(V_t-\lambda)^2-t^2|s_k|^2][(V_b-\lambda)^2-t^2|s_k|^2] + t_\perp^2(V_t-\lambda)(V_b-\lambda)=0, \quad (2)$$

where $s_k=1+e^{i\bar{k}.\bar{a_1}}+e^{i\bar{k}.\bar{a_2}}$, $\bar{a_1}$ and $\bar{a_2}$ are lattice vectors in graphene. In Fig. 1(d), we plot the rate of change of B_e for different directions in the (V_t,V_b) space in polar coordinates with $\theta=\tan^{-1}(V_t/V_b)$. This clearly shows that the rate is maximum (=1) along $V_t=V_b+V_0$, which is essentially the constant band gap locus. As we deviate from this direction, the rate degrades from 1 with minimum along $V_t=-V_b$, leading to the poor subthreshold slope along antisymmetric bias case. As observed from Fig. 1(d), this is a fairly generic result for a large variety of points in the subthreshold region.

We now consider a chemically undoped long channel BLG MOSFET with metal source and drain having low drain bias. The drain current is assumed to be completely dominated by the thermionic carriers, neglecting tunneling. Under these approximations, the electron barrier height B_e is plotted in Fig. 2(a) as a function of V_t and V_b. In the same plot, we also show a number of possible paths p from transistor off state (labeled X_p points) to on state (labeled Y_p points).

Due to the ambipolar nature of the device, it is important to select the appropriate off state for the device. The total integrated carrier density ($N=N_e+N_h$) is shown in Fig. 2(b) in the (V_t,V_b) space to help choose the appropriate set of off state points. In Fig. 2(a), $X_{1,4}$ corresponds to the point of maximum band gap in that range. X_2 corresponds to the maximum electron barrier height though it reduces the hole barrier height, hence increasing N. X_3 is an intermediate point with symmetric electron and hole barrier heights. We

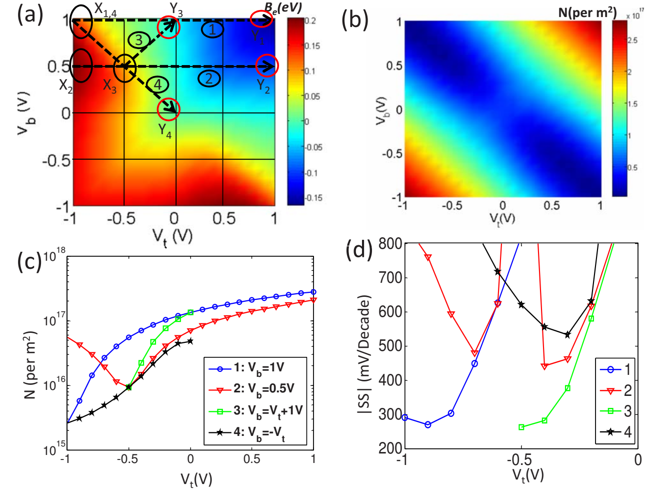

FIG. 2. (Color online) (a) Electron barrier height B_e as a function of V_t and V_b. The four different off to on state arrow paths are numbered as (1)–(4). (b) Integrated carrier density (N) as a function of V_t and V_b. (c) N along the different off to on paths (d) The absolute values of the computed subthreshold slopes for the paths (1)–(4) without any nonideality.

now compare the characteristics among these off to on paths shown in Fig. 2(a), namely (1): V_b is fixed at 1 V and V_t is varied from -1 to 1 V, (2): V_b is fixed at 0.5 V and V_t is varied from -1 to 1 V, (3): $V_b=V_t+1$ V, and V_t is varied from -1 to 0 V, which is an almost constant band gap operation (with $E_g\approx 0.17$ eV), (4): $V_b=-V_t$ and V_t is varied from -1 to 0 V, which is the maximum band gap tunability path. It should be noted that (1) and (2) correspond to single gate operation with back gate at fixed bias. On the other hand, (3) and (4) correspond to double gate operation, although unconventional, with top and bottom gates at different biases. The conventional double gate operation with $V_t=V_b$ is of little significance due to zero band gap. Figure 2(c) shows N as a function of V_t in these four cases. It is clearly observed that the best on/off ratio obtained is ~100. Also, path (1) and (4) will have lower off current than (2) and (3), which is also expected from the Fig. 2(b). Path (4) is found to have low on/off ratio due to the poor tunability of barrier heights (though band gap tunability is maximum) in the antisymmetric case.

To get insights into the above, we find the drain current in a long channel transistor as $I_d=qN\tau$, where τ is the transport factor. In a MOSFET configuration, τ is a weak function of gate voltage. Hence, the subthreshold slope is $SS=\ln(10)\times(\partial V_t/\partial \ln(I_d))\approx \ln(10)(\partial V_t/\partial \ln(N))$. In Fig. 2(d), the computed subthreshold slopes are plotted for the paths (1)–(4) with varying V_t. Note that, unlike conventional MOSFET, the computed subthreshold slope is not independent of gate bias in the BLG transistor.

Analytically, we can convert the summation used in Eq. (1) into an integral to obtain N,

$$N=2\left\{\int_{-\infty}^{E_v} D_v(E)[1-f(E)]dE+\int_{E_c}^{\infty} D_c(E)f(E)dE\right\}, \quad (3)$$

where only one band is assumed to contribute in the conduction band (CB) and the valence band (VB). $E_{v,c}$ are the VB_{max} and CB_{min} obtained from the self-consistent electrostatics. $D_{v,c}$ are the two-dimensional DOS of VB and CB,

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respectively, and we replace them by an average DOS D using the fact that close to band edge, $D_{v,c}$ change much slowly as compared to Fermi function. Utilizing CB-VB symmetry, we find

$$N = 2k_BTD \ln[(1 + e^{-B'_e})(1 + e^{-B'_h})], \quad (4)$$

where $B'_e = B_e/k_BT = (E_c - \mu)/k_BT$ and $B_h = B_h/k_BT = (\mu - E_v)/k_BT$. As D is weakly dependent on V_t, we obtain

$$SS = -\ln(10)\frac{k_BT\kappa \ln(\kappa)}{\left[e^{-B'_e}\frac{\partial B_e}{\partial V_t} + e^{-B'_h}\frac{\partial B_h}{\partial V_t} + e^{-E'_g}\frac{\partial E_g}{\partial V_t}\right]}, \quad (5)$$

where $\kappa = (1 + e^{-B'_e})(1 + e^{-B'_h})$ and $E'_g = E_g/k_BT = (B_e + B_h)/k_BT$. In a conventional Si MOSFET, in the subthreshold region, $B'_e, B'_h \gg 0$, E_g is constant and no gate field screening occurs due to small carrier density ($|\partial B_{e,h}/q\partial V_t| = 1$). Under these conditions, it is straight forward to show that SS reduces to $\ln(10)(k_BT/q)$ (=60 mV/decade at T=300K). Unfortunately, for bilayer graphene, these three conditions are never satisfied simultaneously which degrades the subthreshold slope. To open up a band gap in BLG, unlike conventional semiconductor, we need to apply significantly large fields at the two gates. This in turn causes a large number of carriers to be present in the device, even in subthreshold [though it is possible that the overall device is close to neutral, like in the case of $V_t = -V_b$, Fig. 1(c)]. These carriers cause a strong screening of the gate field and hence, a reduction in the derivatives in the denominator of Eq. (5). Thus, even if we create a significant band gap using vertical field, the carriers thus generated degrade the subthreshold slope.

In the antisymmetric bias case [path (4)], using $B_e = B_h = E_g/2$, we find from Eq. (5) that the SS limit reduces to $60/|\partial B_e/q\partial V_t|$. As $|\partial B_e/q\partial V_t|$ is intrinsically small in this direction [see Fig. 1(d)], SS degrades significantly. On the other hand, along the constant band gap paths (e.g., path 3), the SS limit again reduces to $60/|\partial B_e/q\partial V_t|$. However, in this case, the strong screening due to large number of carriers reduces the denominator, limiting SS much above Boltzmann limit. Finally, we have numerically performed a global search in the (V_t, V_b) space with $|V_{t,b}| \leq 1$ V, which shows that the best SS for all possible constant band gap paths is around 200 mV/decade, whereas along all possible constant V_b paths is around 275 mV/decade.

Thus, we find that along the constant band gap loci, the fundamental limit of SS arising from the bias dependent electronic structure is 60 mV/decade [see Fig. 1(d)], but the screening due to the presence of large number of carriers arising from the unavoidable gate field degrades the subthreshold slope significantly. However, as the operating condition moves away from this direction, both the electronic structure as well as the screening effect play major roles to degrade SS. Nonetheless, the shown subthreshold slope limits are significantly less than the most recent experimental data reported[10] where the extracted value of the minimum subthreshold slope is ~550 mV/decade. This clearly shows that there is room for significant technological improvement in bilayer graphene, including efforts in improving transport derived band gap, effective oxide thickness, and choosing the optimized path from on state to off state.

In conclusion, we have developed a coupled self-consistent Poisson-bandstructure solver for dual gated bilayer graphene and benchmarked against published experimental data. It has been shown that the bias dependent electronic structure and the self-consistent electrostatics limit the subthreshold slope obtained in such a transistor well above the Boltzmann limit, but again much below the results experimentally shown till date.

K. M. and N. B. would like to sincerely acknowledge the support from the Ministry of Communication and Information Technology (MCIT), and the Department of Science and Technology (DST), government of India.

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