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Graphene based transversal-gated field effect transistor due to band gap modulation

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1. Introduction

Neutral graphene is a zero band gap semimetal whose valence and conduction bands touch at the Brillouin zone corners. This fact makes pure graphene unsuitable for use in electronic device applications. Recently, the field has witnessed a concerted effort in the study of gapped graphene, e.g. via epitaxial growth on substrates [1], and application of top and back-gates (in graphene bilayers) [2]. Another promising method is via quantum confinement, e.g. in quasi one-dimensional strips of graphene known as graphene nanoribbons (GNRs). The energy band gap of GNRs is a strong function of their width and edge profile. For example, GNRs with armchair edges (AGNRs) generally exhibit semiconducting behavior, whilst zigzag GNRs are always metallic. Recently, it was also shown that the band structure of monolayer AGNRs can be varied by applying transversal potential [3]. With exploiting this effect, in this work, we introduce a transversal field effect transistor (FET) device (see Fig. 1). Unlike the conventional FET device whose gates are fabricated on top and bottom of the channel, transversal field effect transistors have the gates on the sides. Therefore, the channel layers can be stacked vertically as shown in Fig. 1(a), thus allowing multiple channels controlled by a single set of gates, resulting in a highly compact integration compared to conventional FET structure.

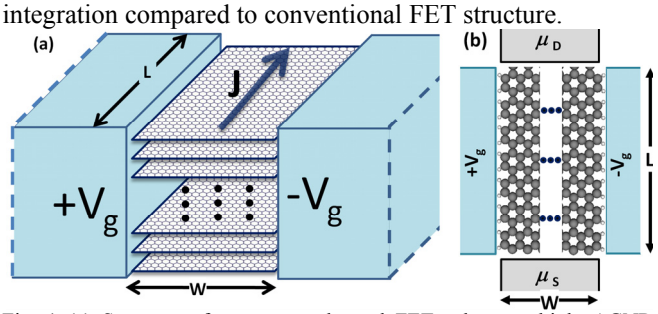

Fig. 1 (a) Structure of a transversal-gated FET, where multiple AGNR channels are stacked vertically. (b) Top-view of a channel layer - AGNR with two side gates of opposite polarity. We assume a linear potential drop across the transverse direction of the structure. Source-drain bias is $\mu_{sd}=\mu_S-\mu_D$.

2. Simulation Model

We employ the nearest neighbor pi-orbital tight binding model [4] to study the electronics structure of a GNR. The Hamiltonian of a GNR is given by $H=\sum_n V_n a_n^+ a_n - \sum_{n,m} t_{n,m} a_n^+ a_m$, where V_n is the onsite energy at site n including the potential across through the channel caused by the transversal gates, and $t_{n,m}=t\approx 3$eV is the hopping energy between two bonded atoms m and n. Here $a_n^+(a_n)$ refers to the electron creation (annihilation) operator at atom n. The electron transport of the GNR is studied using the non-equilibrium Green's function (NEGF) formalism. The transmission across the GNR at energy E is $T(E)=trace\left[\Gamma_S(E)G^r(E)\Gamma_S(E)G^r(E)^+\right]$, where G^r is the retarded Green's Function of the device region, and $\Gamma_{S(D)}$ denotes the coupling between the source (drain) with the GNRs. The current density across GNRs is given by $J=(e/h)\int_{-\infty}^{\infty}T(E)\left[f_S(E)-f_D(E)\right]dE/W$, where $f_{S(D)}$ is the source (drain) Fermi distribution function, and W is the GNR width. To understand the fundamental device physics in this work, we assumed that the Laplace potential linearly across the transverse direction of the AGNR, and the vertical distance between nearest dimmers in the AGNR is represented by a_y=0.1247nm. Unless otherwise stated, in all our simulation we used the channel length, L=14.4nm.

3. Results and Discussion

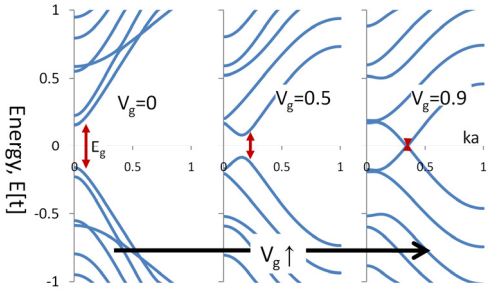

Fig. 2: Band structure variation of AGNRs with increasing gate potential, V_g. The minimum distance between the valence band and conduction band decreases as V_g increases. Here, the AGNR width W=13a_y.

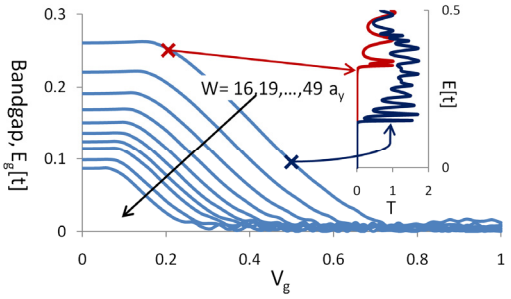

Fig. 3: Band gap variation with increasing V_g for different widths. The inset shows the conductance when U_g=0.2 and 0.5 [W=16a_y]. The conduction gap is decreased when V_g=0.5.

Firstly, we study the variation of the band structure of AGNRs with transverse-gate potential, V_g. Below, we considered semiconducting AGNRs with type I (total number of dimmers N_a=3p+1, where p is an integer) [5], since these AGNRs have the largest band gap when V_g=0. Fig. 2 shows the changes in band structure as V_g increases (throughout this work, V_g is expressed in units of t/e). The minimum separation between the conduction and valence band, i.e. the

band gap (E_g), changes with increasing V_g, due to the spectral shift of the conduction and valence band states at the edges. In Fig. 3, the variation of the band gap with increasing V_g for AGNRs with different widths are studied. We found that under a sufficiently high V_g, the gap is close to zero, i.e. $E_g \rightarrow 0$. This indicates that AGNR from a semiconductor transits to metallic by introducing the transversal electrical field. [3] It is also found that for larger widths W, E_g starts to decrease and approaches zero at lower V_g. Furthermore, the inset of Fig. 3 shows the change in conduction gap of the devices proposed in Fig. 1 under V_g=0.2 and 0.5 when W=16a_y. As V_g increases the conduction gap decreases corresponding to the decrease in E_g. As the conduction gap decreases the AGNR becomes more conducting, resulting in higher source-drain current (J_{SD}).

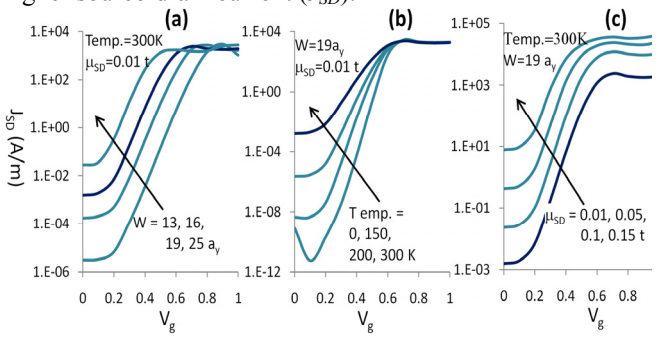

Fig. 4: Source drain linear current density, J_{ds} –U_g for varying (a) AGNR width W, (b) temperature *Temp.*, and (c) source-drain bias μ_{sd}. Unless otherwise stated: *Temp.*=300K, W=19 a_y; and μ_{SD}=0.01t.

In Fig. 4 we present the variation of simulated J_{SD} with increasing V_g under various conditions. All devices present the transistor behaviors with the ON and OFF states with the different V_g caused by bandgap modulation under the transversal electrical field. Fig. 4(a) shows the effect of AGNR width on J_{SD}. As the width increases, the E_g under V_g=0 decreases, resulting in lower OFF-J_{SD}. On the other hand, the ON-J_{SD} remains same under different W. It is because at ON-state, $E_g \approx 0$ regardless of W. Moreover, the on-state is achieved at lower V_g for devices with larger width, since for larger W, the E_g begins decreasing at lower V_g [cf., Fig. 3]. Next, we investigate the effect of temperature (*Temp.*) on J_{SD} as shown in Fig. 4(b). Due to the spreading of the Fermi distribution function, under the high temperature, the OFF-J_{SD} increases, and hence the performance of the transistor degrads. Fig. 4(c) shows the effect of source-drain bias, $(\mu_S-\mu_D)/e$. As the bias increases, the conduction window is widened and thus, more electrons are transported in the device, resulting in higher OFF-currents and ON-currents.

Finally, we explore the edge vacancy effects on device characteristics. Interestingly, we find that the subthreshold slope (SS) can be further decreased, by defect engineering at the edges. Referring to Fig. 5, when we introduce vacancies at the top-edge (35%), the conduction gap increases in the OFF-state. It is because type I AGNR has the largest bandgap compared to the two types, and hence any fluctuation on the edge will increase the bandgap. However as V_g is increased, the conduction gap decreases at a higher rate in the disordered structure. This results in a lower OFF-J_{SD} and smaller SS. The J_{SD} curve with vacancies at the top edge is shown in Fig. 6. As predicted, the OFF-current and the SS are lower for the disordered AGNR transversal gate FETs and the ON-state can be reached at lower V compared to the smooth-edge one. However, vacancies also suppress the magnitude of the conductance due to the scattering processes as shown in Fig. 6. Therefore, a careful engineering of the vacancies can optimize the performance of the transistor.

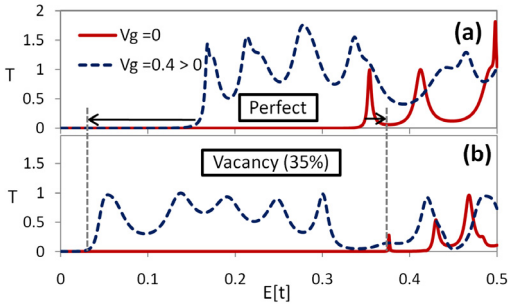

Fig. 5: The effect of vacancies at the top edge in modifying the conduction gap. (a) Conductance of a perfect structure, (b) conductance of disordered structure. Vacancies increase (decrease) the conduction gap when V_g=0 (V_g is high). [W=19a_y, *Temp.*=300K]

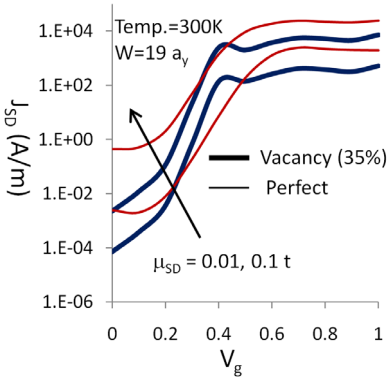

Fig 6: Source-drain linear current density, J_{ds}–U_g for varying source-drain bias, μ_{sd}. Thick (thin) lines show the variation for a disordered (perfect) structure. The slope is enhanced due to vacancies. However, the off current is reduced.

4. Conclusion

In summary, we have explored the possibility and fundamental physics of a transversal-gated FET in which an asymmetric electrochemical potential is applied to the lateral edges of a monolayer AGNR. This potential causes a reduction in the band gap of the AGNR, thus resulting in larger current flow across the device. We found that the device performance can be improved by introducing vacancies at the top edge of the structure. Engineering of the device width and vacancies play an important role in optimizing the device performance.

References

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