EE230C Final Project: Monolayer Graphene

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i.

The experimental performance of several sub-100 nm graphene transistors were demonstrated by Wu for RF purposes[1]. The topology of these graphene devices is shown in Figure 1. The current-voltage characteristics of the 70 nm FETs were measured at both room temperature and low temperature. The performance of the FETs were also modeled, and Figure 2a and 2b shows a comparison of the experimental and modeled current I_d vs the gate voltage V_g and the drain voltage V_d , respectively.

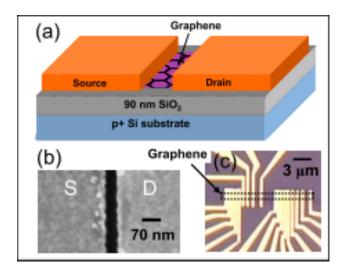


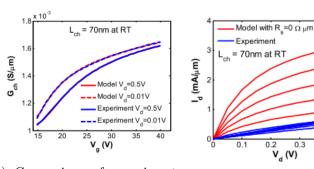
Figure 1: (a) Schematic view of Wu's back-gated graphene FET, (b) SEM image of metal contacts of a 70nm device and (c) optical image of the fabricated devices.

Experimental data of the contact resistance was also collected at different temperatures, as seen in Figure 3. For the 70 nm device, contact resistance for electrons was around 275 $\Omega - \mu m$. Mobility data vs temperature was also collected, shown in Figure 4.

Additionally, Meric et al [2] took a comprehensive look at channel-length scaling of graphene FETs, including several with channel lengths under 100 nm. Their graphene FET design is similar to Wu's, and is shown in Figure 5.

ii.

To calculate the current-voltage characteristics, we first derived the bandstructure of graphene. The Hamiltonian matrix is first constructed, and the eigenvalues are determined computationally. Using the six-band tight-binding model with bulk graphene parameters from Boykin et al [3], the p_z, d_{yz}, d_{zx} bands are included in the calculation to make a 6 by 6 Hamiltonian of the form:



- (a) Comparison of experiment and model of the transfer char- (b) Modeled output characterisacteristics.
 - tics with $R_s = 0$ vs experiment.

Figure 2: Measurements by Wu of 70 nm device at room temperature

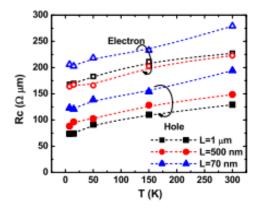


Figure 3: Contact resistance R_c vs T from devices with different channel length, from 1 μ m to 70 nm.

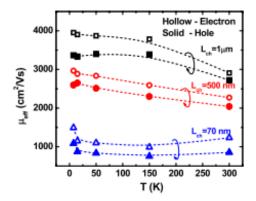
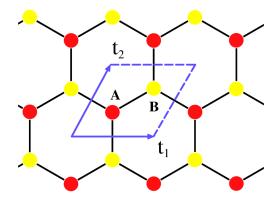


Figure 4: Effective electron and hole mobility μ_{eff} vs T from devices with different channel length, from 1 μ m to 70 nm.

$$H = H_{on} + H_{off}e^{i\vec{k}\vec{a_1}} + H_{off}^Te^{-i\vec{k}\vec{a_1}} + H_{off}e^{i\vec{k}\vec{a_2}} + H_{off}^Te^{-i\vec{k}\vec{a_2}}$$

 $H=H_{on}+H_{off}e^{i\vec{k}\vec{a_1}}+H_{off}^Te^{-i\vec{k}\vec{a_1}}+H_{off}e^{i\vec{k}\vec{a_2}}+H_{off}^Te^{-i\vec{k}\vec{a_2}}$ Here, the vectors $\vec{a_1}$ and $\vec{a_2}$ represent the basis vectors for the graphene unit cell, as denoted in Figure 1. The \vec{k} is the momentum vector, which we allow to take values over the entire first brillouin zone.



Using the method of Linear Combination of Atomic Orbitals as described in Slater Koster To derive the current-voltage characteristics of these transistors, we proceed from the fundamental equation:

$$I_d = -2ew(\sum_{k_x > 0, ky} f_k v_k - \sum_{k_x < 0, ky} f_k v_k)$$

This includes back-scattering of electrons going back over the barrier from the drain. We recall the expressions for f_k and v_k :

$$f_k = \frac{1}{1 + exp(\frac{\mathcal{E}_k(k_x, k_y) - \mu}{k_P T})}, \quad v_k = \frac{1}{\hbar} \nabla_k(E) = \frac{1}{\hbar} (\frac{dE}{dk_x} + \frac{dE}{dk_y})$$

Here, since we are working from the numerical values of the rigorous bandstructure, v_k is calculated numerically from the gradient of E_k with respect to both k_x and k_y .

After deriving the bandstructure, the current can be determined computationally after converting the sum into a double integral by taking the limit of k_x and k_y to 0 and normalizing by $\frac{1}{4\pi^2}$:

$$\sum_{k_x>0,ky}f_kv_k=\int_0^\infty dk_xdk_yv_kf_k=\int_0^\infty \frac{1}{4\pi^2}dk_xdk_y\frac{1}{1+exp(\frac{\mathcal{E}_k-\mu_S}{k_BT})}\frac{1}{\hbar}\nabla_k(E)$$

With the corresponding expression for current from electrons going back over the barrier:

$$\sum_{k_x < 0, ky} f_k v_k = \int_{-\infty}^0 dk_x dk_y v_k f_k = \int_{-\infty}^0 \frac{1}{4\pi^2} dk_x dk_y \frac{1}{1 + exp(\frac{\mathcal{E}_k - \mu_D}{k_B T})} \frac{1}{\hbar} \nabla_k(E)$$

This takes care of current from electrons. To derive the total current, we must also take the hole current into account, using the similar formula

$$I_{D-holes} = 2ew(\sum_{k_x < 0, ky} f_k v_k - \sum_{k_x > 0, ky} f_k v_k)$$

because holes flow the opposite direction of electrons. While the velocity v_k is calculated the same for holes, the Fermi function f_k changes:

$$f_{kholes} = 1 - f_{kelectrons}$$

Then, proceeding the same way, the hole current is calculated and the total current I_d is

$$I_d = I_{delectrons} + I_{dholes}$$

This, however, only takes care of variation with the drain voltage V_d . To implement gate control by the gate voltage V_g , the potential at the top of the barrier between source and drain is self-consistently with the number of carriers at the top of the barrier. For this model, charges in the channel are provided through thermionic emission from the source and drain contacts. Both electron and hole charges are taken into account to explain both positive and negative bias behavior.

At equilibrium the concentration of carriers is the following:

$$N0 = \int_{-\infty}^{\infty} D(E)f(E - Ef)dE$$

where D(E) is the density of states calculated from the band structure, and f(E) is the fermi function at that energy level. This is used as an initial guess for the self consistent solve. We use the following equations, as described by [5].

1.
$$U_{TOB} = q\phi(\frac{C_G}{C_T} + \frac{C_D}{C_T}) + q^2 \frac{N - N_0}{C_t}$$

2.
$$N = \int_{-\infty}^{\infty} D(E) f(E + U_{TOB} - \mu_s) + \int_{-\infty}^{\infty} D(E) f(E + U_{TOB} - \mu_d)$$

The contribution for holes in the total carrier is added by substituting the fermi functions and energies as described above. During all further models, we approximate that the source side potential, μ_s , is grounded, and all other potentials are referenced from that point (μ_d , μ_g , etc.), making $\mu_s = 0$.

For calculation of the gate capacitance, we calculate capacitances based on a 90nm SiO2 structure as described in by [1]. The drain to channel coupling capacitance is left as a fitting parameter, and is used to approximate the effects of DIBL and other short channel effects.

Figure showing DIBL plots*

iii.

The injection velocity is defined as follows:

$$v_{inj} = \frac{\sum_{k_x > 0, ky} f_k v_k}{\sum_{k_x > 0, ky} f_k}$$

As before, this expression can be converted into an integral expression which includes E_k , when determining the Fermi function f_k , and $\nabla_k(E)$, when determining the velocity v_k . Computing the integral as before using the rigorous bandstructure determined computationally, we obtain a thermal velocity of v_{th} =.

Graphene is notable because, due to the non-parabolic shape of its bandstructure, one cannot obtain an effective mass[4] using the conventional definition $m^* = \hbar^2 (\frac{d^2 E(k)}{dk^2})^{-1}$. Instead we proceed with an alternative definition $m^* = \hbar^2 k (\frac{dE(k)}{dk})^{-1}$. This is based on the linear bandstructure of graphene in a small region around the Dirac point. Using the usual effective mass approximation that $E = \frac{\hbar^2 k_x^2}{2m^*}$

From the rigorous bandstructure, the injection velocity was determined to be

iv.

 $\mathbf{v}.$

Efficacy of device

References

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- [3] Boykin, T. et al., "Accurate six-band nearest-neighbor tight-binding model for the π bands of bulk graphene and graphene nanoribbons.". Journal of Applied Physics, 109.10, (2011).
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