Graphene switches: electronics to electron 'optics'

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The unique bandstructure of graphene generates spectacular properties, record electronic and thermal conductivities for suspended samples, and electronic analogs of optical metamaterials. These properties arise from graphene's 2D geometry, its linear E-k and non-dispersive trajectories at finite voltages, lack of a band-gap leading to Zener/Klein tunnelling, and its pseudospin degrees of freedom. We discuss how to include these effects in a unified transport formalism.

QUANTUM FLOW OF ELECTRONS

We use a single orbital tight-binding model for the graphene Hamiltonian within the non-equilibrium Green's function (NEGF) formalism, the current involving the modal spectrum and transmission integrated within a voltage window. We use partial inversion to calculate the Green's functions recursively, simulating upto 200nm x 600nm, ie, 5 million atom devices. Experimental conductivities and inverter characteristics can be readily correlated with these calculations. Fig.1 shows the current density plotted for a 100nm x 100nm structure, showing lensless focusing of electrons at a PN junction [1], one of the gate voltages acting as a negative refractive index in an electronic analog of Snell's law. Note that there are some standing waves on the left set up by the finite width. Nonetheless, we can see the entire gamut of electronic trajectories, from total internal reflection to Klein and anti-Klein tunneling in mono and bilayer junctions. We can use this to design pseudospin transistors with high ON-OFF ratios and subthermal switching, for which there is now experimental evidence. The code can be sped up by parallelizing the outer voltage and inner current loops. Together with O(N) banded system solvers for fast partial matrix inversion, we see significant further speed-up.

SCATTERING WITHIN GRAPHENE

Within an atomistic NEGF formalism, we can add scattering from impurity distributions and phonons with numerically computed densities of states. The conductivity shows sidebands signalling the onset of inter-subband scattering, in excellent quantitative agreement with experiments from Phil Kim's group at Columbia (Fig. 2).

EDGES CAN BE IMPORTANT

For ultrathin nanoribbons, edges are in fact, critical. We pointed out that dimerization at the edge of armchair ribbons drives them towards a benzene-like structure with 3.5% strain, and eliminate metallicity [2]. Furthermore, edge roughness removes chiral signatures [3], allowing us to control bandstructure with width alone [4] and design wide-narrow-wide structures with superior electrostatics and quasi-ohmic contacts. To handle these effects, we need a Hamiltonian that can handle strain and reconstruction. We do that in two ways – (a) by expanding to a larger sp^3 basis set using non-orthogonal atomistic Extended Huckel Theory for predictive edge chemistry; and (b) by reverting to phenomenological tight-binding with next nearest neighbour interactions, parametrized by CT White. The results from both methods are in excellent agreement (Fig.3).

REMOVING EDGE SCATTERING FOR WIDE SHEETS

The need for computational speed is to simulate large structures that eliminate edge effects, since standing waves tend to overwhelm the transport physics. A better approach is to implement open boundary conditions on a finite segment. We accomplish this in four ways: (a) for infinitely wide contacts and channel, we can use k-space formalism in the transverse direction, allowing us to recover the bulk density of states (Fig. 4) and the PN junction conductance (Fig. 5) out of just a short 1nm x 1nm segment, eliminating the quantization signatures from Fig. 3; (b) by adding virtual leads on each side recursively, which takes the electrons away irreversibly (Fig. 6); (c) by 'scooping', ie, treating the segment as part of an infinite structure, for which we can calculate the Green's function of the unperturbed segment and

reverse-engineer the corresponding self-energy. This is a technique borrowed from the area of boundary value mathematics, building on past work by Inglesfeld, Baraff and Schluter. The above three techniques are general and work for any shaped source/drain contacts at equilibrium (figuring out the nonequilibrium correlation functions is trickier). Finally, (d) by adding an incoherent scattering term at the edges. Ideally this should be energy dependent for current conservation, but we already see in Fig. 7 how edge reflections are removed using this approach.

ACKNOWLEDGEMENT

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REFERENCES

1. R. Sajjad and A. W. Ghosh, *High efficiency switching using graphene based electron optics*, Appl. Phys. Lett. **99**, 123101 (2011).

2. F. Tseng, D. Unluer, M. R. Stan and A. W. Ghosh, *Graphene Nanoribbons: from chemistry to circuits*, invited book chapter (Graphene Nanoelectronics: Metrology, Synthesis, Properties and Applications, Ed. H. Raza, Springer Series in Materials Science).

3. F. Tseng, D. Unluer, K. Holcomb, M. Stan and A. W. Ghosh, *Diluted chirality dependence in edge rough graphene nanoribbon field-effect transistors*, Appl. Phys. Lett. **94**, 223112 (2009).

4. D. Unluer, F. Tseng, A. W. Ghosh, M. R. Stan, *Monolithically Patterned Wide-Narrow-Wide All-Graphene Devices*, IEEE Trans. Nano **10**, 931 (2011).

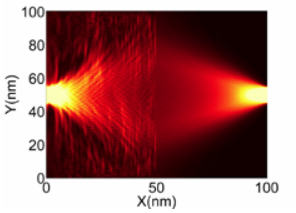

Fig1. Focusing of electrons at a PN junction, driven by Klein tunneling with conserved pseudospins (model with 380,000 atoms). Edge reflections show standing waves on the left.

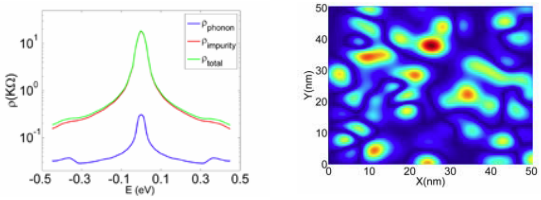

Fig2. Atomistic treatment of bilayer graphene conductivity (left), including (right) ensemble averaged gaussian impurity scattering potentials (n_{imp} = 2 x 10^{11} cm^{-2}, right) in a 50 x 50nm sheet and phonon scattering through Fermi's Golden rule with atomistically calculated density of states.

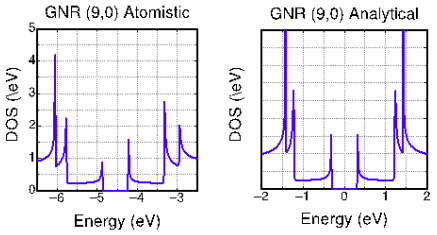

Fig3. (Left) Atomistic Extended Huckel and (Right) parametrized tight binding density of states for (9,0) ribbon.

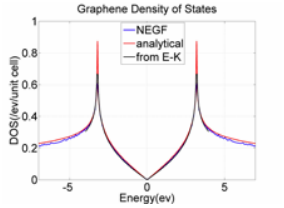

Fig4. Density of states of graphene sheet obtained analytically, obtained from numerical sums over the E-k states, and obtained from atomistic NEGF with k-space applied to a very small (1nm x 1nm) region.

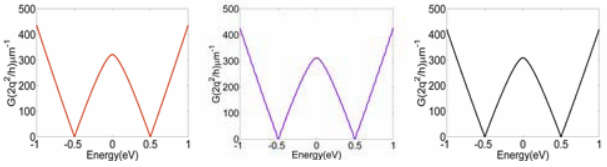

Fig5. (Left) Analytical conductance of infinitely wide PN junction, vs numerical atomistic results for (middle) finite 100nm x 100 nm sheet, and (right) 1nm x 1nm sheet with k-space transmission sums in the transverse direction.

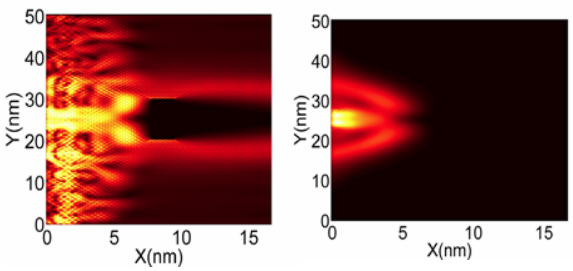

Fig. 6 Electrons reflecting near the source of a PN junction, eliminated with open boundary conditions through a recursively calculated self-energy. An added tunnel barrier is engineered in the middle for high ON-OFF ratios [1]

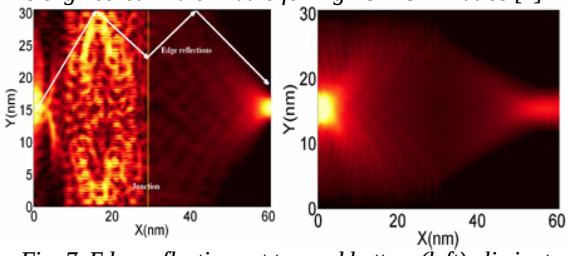

Fig. 7. Edge reflections at top and bottom (left) eliminated by adding incoherent scattering.