Electro-Thermal Transport in Graphene Devices

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We have used simulations verified by extensive experimental data to understand the (coupled) electrical and thermal behavior of graphene transistors and interconnects. Using infrared thermal imaging [1] we uncovered that graphene transistors (GFETs) heat up non-uniformly during high-field operation, due to varying carrier density and E-field along the channel. A hot spot forms at the location of maximum field (minimum carrier density), and its position depends on the applied voltages (Fig. 1) [1].

In addition, using scanning Joule expansion microscopy (SJEM) [2] we have uncovered that thermoelectric effects become important at graphenemetal contacts. For instance, approximately one-third of the temperature rise at graphene contacts is controlled by Peltier effects and about two-thirds by Joule effects, but this proportion will shift in favor of the Peltier effect as graphene contact resistance is improved in future technologies [2].

SELF-CONSISTENT DEVICE MODELLING

We have developed self-consistent GFET simulations coupling the drift-diffusion equations, Poisson equation, heat diffusion equation, and thermoelectric contact effects [1-5]. These models can simultaneously fit (and extract) graphene mobility, contact resistance, Seebeck effect, thermal conductivity, and thermal conductance to the substrate. The models are best applied in devices larger than the electron and phonon mean free paths in graphene (20-100 nm), where most experimental data are available.

We have recently extended this work to understand current saturation in sub-micron GFETs on SiO₂/Si substrates (Figs. 2-3). We uncovered that strong self-heating limits the maximum current to ~1 mA/µm, but self-heating also "helps" achieve better current saturation and lower output conductance ($g_o = \partial I/\partial V_{ds}$) which is important for amplifier gain [3]. Interestingly, devices shorter than about 0.5 µm benefit from heat sinking at the contacts, which simultaneously reduces their current saturation [3].

GRAIN BOUNDARIES & SUSPENDED GRAPHENE

We have also used non-equilibrium Green's functions (NEGF) to investigate heat flow at grain boundaries (GBs) in graphene grown by chemical vapour deposition (CVD). We found that "not all defects are created equal", in other words that line defects scatter phonons more strongly than GBs (Fig. 4) [4].

Most recently, we have succeeded in suspending graphene devices to examine the extreme case of coupled electro-thermal behaviour at high field [5] (Figs. 5-6). We uncovered the *intrinsic* drift velocity saturation in graphene, as well as the thermal conductivity k scaling up to ~2000 K (Fig. 6). Interestingly, graphene k decreases as $\sim T^{-1.7}$ while graphite k as $\sim T^{-1.1}$ at high temperature, likely due to a stronger second-order three-phonon scattering which must be further investigated.

CONCLUSION

Graphene devices present an interesting set of challenges, due to their high in-plane mobility and thermal conductivity, but poor thermal coupling to the environment [6]. Our simulations coupled with experiments have shed physical insight into such coupled behaviour, particularly at high-fields typical of modern devices. Challenges remain in understanding, e.g., the behaviour of GFETs on "well-matched" substrates such as BN, and on highly insulating substrates such as plastics.

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Fig. 1. Infrared (IR) thermal imaging of graphene field-effect transistor (GFET) during operation, from [1]. The figure is a sequence of IR images taken at varying V_{GS} as labeled, and $V_{DS} = 12$ V. A hot spot forms at the location of highest field, and "moves" along the channel as the voltages are varied [1].







Fig. 3. Simulated thermal transient of a GFET (see Fig 2), (a) without and (b) with a capping layer. (c) Thermal time constants of a GFET are in the range 30-300 ns, much slower than electrical switching time constants [3].



Fig. 4. (a) Schematic of grain boundary (GB) and (b) line defect (LD) in graphene. (c) Computed thermal conductivity of graphene with GBs and LDs, as a function of grain size (or average distance between defects) $\ell_{\rm G}$ [4].



Fig. 5. (a-b) Schematic and experimental suspended graphene, the extreme case of electrical and thermal coupled transport at high field. (c) Experimental data across 15 suspended devices (red: exfoliated, blue: CVD-grown graphene). (d) Simulation of suspended devices explaining the different types of behavior seen at high-field [5].



Fig. 6. Summary of *intrinsic* high-field properties of suspended graphene across 15 samples: (a) saturation velocity, (b) thermal conductivity at 1000 K, (c) thermal conductivity k scaling at high temperature, and comparison to previous data and to graphite [6]. Graphene k appears to drop more steeply at high T than graphite. See ref. [5] for in-depth discussion.