Supplementary Information: Nanoscale control of graphene electrodes

C.S. Lau,[a] J.A. Mol,[*a] J.H. Warner[a] and G.A.D. Briggs[a]

[a]Department of Materials , University of Oxford, 16 Parks Road, Oxford OX1 3PH, UK

[*]To whom correspondence should be addressed; E-mail: jan.mol@materials.ox.ac.uk.

Conformal mapping

We calculate the current density by employing the technique of conformal mapping. This maps the complicated boundary conditions of a given geometry to another geometry for which the boundary conditions are simple. The solution of the Laplace equation, which is invariant under transformation, in the transformed geometry may than be inverse-transformed to give the required result.

First, we define the edges of the graphene notch by transforming the Cartesian coordinates (x, y) to the elliptic coordinates (μ, ν) defined by

$$x = \cosh(\mu)\sin(\nu) \quad (1)$$

$$y = \sinh(\mu)\cos(\nu), \quad (2)$$

where μ is a real number and $\nu \in [-\pi/2, \pi/2]$. On the complex plane the relationship is

$$z = \cosh(\zeta + i\pi/2) \quad (3)$$

with $z = x + iy$ and $\zeta = \mu + i\nu$. The graphene notch is contained between the two boundaries $|\nu| \leq \nu_0$ and the width of the narrowest part of the graphene notch, at $\mu = 0$, is $h = 2\sin(\nu_0)$.

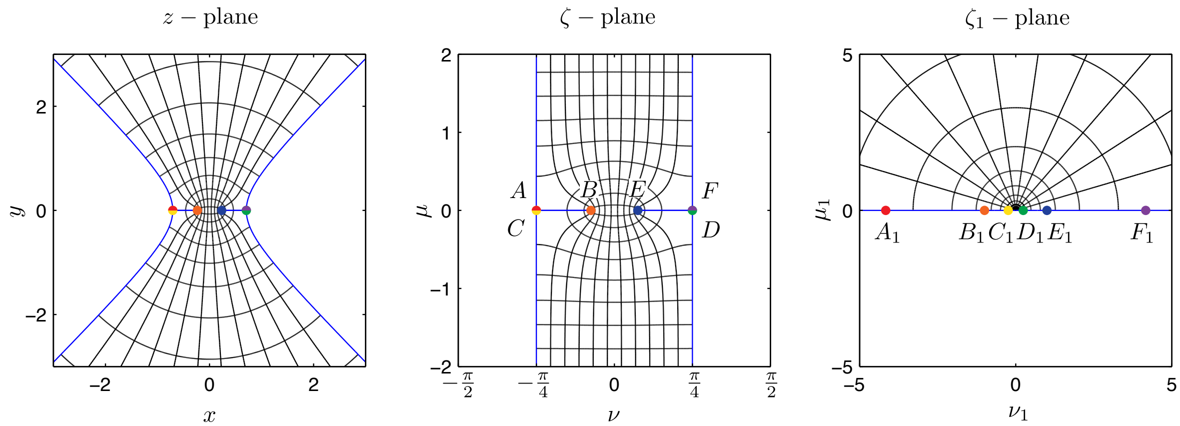

Figure SI1: **Conformal mapping** The complicated boundary conditions for the notched ribbon geometry are mapped on a geometry with simple boundary conditions. The first transformation ,from the z-plane to the ζ-plane, maps the edges of the graphene notched ribbon on two vertical lines corresponding to $|\nu| = \nu_0$. A second transformation maps the left boundary in the ζ-plane, including the void with infinitesimal thickness between A, B, C on the negative real axis of the ζ_1-plane, and the right boundary on the positive real axis of the ζ_1-plane.

Next, the partially formed nano-gap is defined as two voids with infinitesimal thickness extending inwards from the edges of the graphene at the narrowest part of the notch, the vertices of which are indicated as A, B and C for the left void and D, E and F for the right void on the ζ-plane in Fig. SI1. The distance between the two voids in the ζ-plane is $2\omega_0$, so that the width of the graphene between the two voids is $k = 2\sin(\omega_0)$. The Schwarz transformation

$$\zeta = \frac{2\nu_0}{\pi}\tan^{-1} s \pm \nu_0, \tag{4}$$

where the sign of ν_0 corresponds to the sign of ζ_1 and

$$s = \frac{\sqrt{(a^2 - \zeta_1^2)(\zeta_1^2 - 1/a^2)}}{\zeta_1^2 + 1}, \tag{5}$$

with

$$a = \tan\alpha + \sec\alpha, \quad \alpha = \left(1 - \frac{\omega_0}{\nu_0}\right)\frac{\pi}{2}, \tag{6}$$

maps points $A, B, C, \ldots$ on the ζ-plane onto points $A_1, B_1, C_1, \ldots$ along the real axis of the ζ_1-plane. For z contained between the two boundaries $|\nu| \leq \nu_0$, the limit $\mu \to -\infty$ will map onto the origin of the ζ_1-plane and the limit $\mu \to +\infty$ will map onto a semicircle of infinite radius in the upper half ($\zeta_1 \geq 0$) of the ζ_1-plane.

Solutions to the Laplace equation are required to give positive and negative potentials for $\zeta_1 \to +\infty$ ($\mu \to +\infty$) and $\zeta_1 \to 0$ ($\mu \to -\infty$), and have no gradient across the real ζ_1 axis which corresponds to the edges of the graphene. For

$$W = U + iV, \tag{7}$$

where U is the potential function, a solution to the Laplace equation that satisfies these conditions is

$$W = j_0 \ln \zeta_1, \tag{8}$$

and the current density in the z-plane is given by

$$j(z(\zeta_1)) = \left|\frac{dW}{dz}\right| = \left|\frac{d\zeta}{dz}\frac{d\zeta_1}{d\zeta}\frac{dW}{d\zeta_1}\right| = j_0 \left|\frac{1}{\zeta_1}\frac{d\zeta}{dz}\frac{d\zeta_1}{d\zeta}\right| \tag{9}$$

$$= j_0 \frac{1}{\sqrt{\sinh^2 \mu(\zeta_1) + \cos^2 \nu(\zeta_1)}} \left|\frac{\sqrt{(a^2 - \zeta_1^2)(\zeta_1^2 - 1/a^2)}}{\zeta_1^2 - 1}\right|. \tag{10}$$

In the absence of the partially formed nano-gap ($a = 1$) the current density is highest at the edges of narrowest part of the graphene notch ($\mu = 0, |\nu| = \nu_0$). Away from the narrowest part of the notch ($\mu \gg 1$) the current density goes as j_0/μ, where μ approaches the radial distance from the centre of the notch. It is therefore to be expected that the nano-gap will form at the apex of the notch;.

When the nano-gap is partially formed ($a > 1$), j diverges for $\zeta_1 \to 1$ which corresponds to tip of the voids (points B and E). This can be understood as the current having to flow around the voids with infinitesimal thickness.

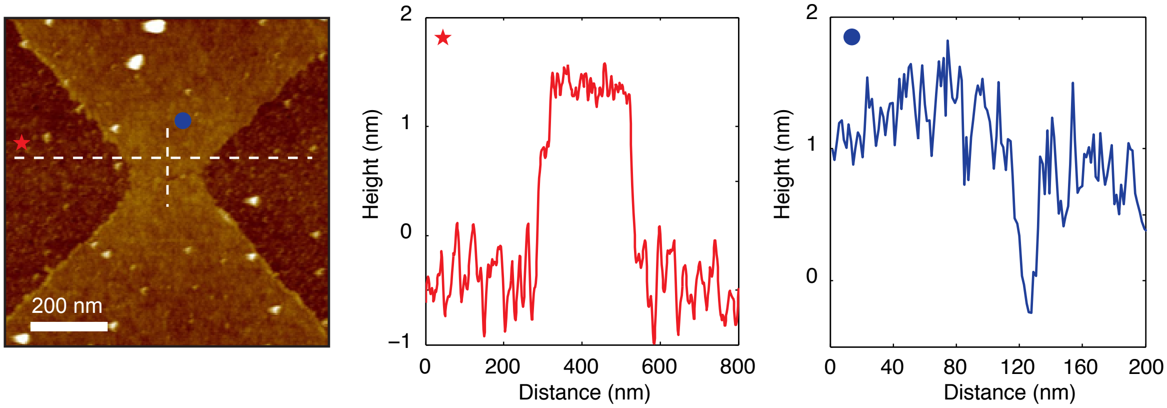

Figure SI2: **Height profiles** The height profiles are measured along the dashed lines in the left panel. The symbols in the left panel indicate the origin of the line profiles in the centre and right panel.

Height profiles

Figure SI2 shows the height profiles alongside and across the nano-gap. The height profile across the nano-gap is measured at the widest part of the gap. At the narrowest part of the gap, where the actual tunnel-junction is formed, the gap-size is too small to resolve with AFM.