Supplementary Information: Deformation and scattering in graphene over substrate steps

T. Low, V. Perebeinos, J. Tersoff and Ph. Avouris
IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA

I. ELASTICITY MODEL

We describe the energy of graphene membrane using a valence force model (VFM) [1]. The Van der Waals interaction with the SiC surface is described by the Lennard-Jones (LJ) 6-12 potential [2].

$$\begin{aligned} E &= \beta_{r1} r_0^{-2} \sum_{i,j\in i} (\delta r_{ij})^2 + \beta_c \sum_{i,j<k\in i} (\delta c_{i,jk})^2 + \beta_v r_0^{-2} \sum_{i,j<k<l\in i} \left(\frac{3 v_{ij} \cdot v_{ik} \times v_{il}}{r_{ij} r_{ik} + r_{ik} r_{il} + r_{il} r_{ij}} \right) \\ &+ \beta_{r2} r_0^{-2} \sum_{i,j<k\in i} (\delta r_{ij})(\delta r_{ik}) + \beta_p \sum_{i,j\in i} |\pi_i \times \pi_j|^2 + \beta_{rc} r_0^{-1} \sum_{i,j\neq k<l\in i} (\delta r_{ij})(\delta c_{i,kl}) \\ &+ \beta_{vdw} \sum_i \int_S \left(\frac{c_0}{|v_i - v'|} \right)^{12} - 2 \left(\frac{c_0}{|v_i - v'|} \right)^6 dv' \\ &\equiv E_{r1} + E_c + E_v + E_{r2} + E_p + E_{rc} + E_{vdw} \end{aligned} \tag{1}$$

where v_i is the atomic position vector of carbon atom i, $v_{ij} = v_j - v_i$ is the bond vector, $r_{ij} = |v_{ij}|$ and $r_0 = 0.142\ nm$. S is the surface of the SiC step. We also define the following,

$$\delta c_{i,jk} = \frac{1}{2} + \frac{v_{ij} \cdot v_{ik}}{r_{ij} r_{ik}} \ , \ \pi_i = 3 \frac{v_{ij} \times v_{ik} + v_{ik} \times v_{il} + v_{il} \times v_{ij}}{r_{ij} r_{ik} + r_{ik} r_{il} + r_{il} r_{ij}} \tag{2}$$

Parameters used for the VFM are [1], $\beta_{r1} = 18.52\,eV$, $\beta_c = 4.087\,eV$, $\beta_v = 1.313\,eV$, $\beta_{r2} = 4.004\,eV$, $\beta_p = 0.008051\,eV$ and $\beta_{rc} = 4.581\,eV$. We assumed $c_0 = 2.7\,r_0$ and $\beta_{vdw} = u_0/a$ for the LJ potentials [2], where $u_0 = 2.4\,meV$ and $a = 3\sqrt{3} r_0^2/4$. Our LJ model would yield an equilibrium interlayer bond distance of $H_{eq} = 2^{-1/6} c_0 \approx 3.4 \mathring{A}$, in good agreement with experiments. The binding energy is given by $E_B = \pi p_0 d_0^2 (2^{5/3}/5 - 2^{2/3}) \approx 40.3\,meV$, in vicinity of reported values in experiments [2, 3]. However, we note its value is still a subject of experimental and theoretical studies [4].

II. TRANSPORT MODEL

The Hamiltonian $\mathcal{H}$ is described by a nearest-neighbor Slater-Koster parameterized sp^3 tight-binding model [5, 6], including the energetically relevant π and σ bands.

$$\mathcal{H} = \sum_{i\alpha} V_i a_{i\alpha}^\dagger a_{i\alpha} + \sum_{ij} \sum_{\alpha\beta} t_{ij,\alpha\beta} a_{i\alpha}^\dagger a_{j\beta} \tag{3}$$

where i, j denotes atomic positions and α, β the atomic orbitals. V_i models the on-site doping and $t_{ij,\alpha\beta}$ describes the energies due to atomic orbital overlaps and are given as,

$$t_{ii,ss} = \epsilon_s \ , \ t_{ii,pp} = \epsilon_p \ , \ t_{ij,sp} = \frac{v_{ij} \cdot p_j}{r_{ij}} \epsilon_{sp} = -t_{ij,ps} \tag{4}$$

$$t_{ij,pp'} = \frac{v_{ij} \cdot p_i}{r_{ij}} \frac{v_{ij} \cdot p'_j}{r_{ij}} \epsilon_{pp}^\sigma + \frac{v_{ij} \times p_i}{r_{ij}} \frac{v_{ij} \times p'_j}{r_{ij}} \frac{(v_{ij} \times p_i) \cdot (v_{ij} \times p'_j)}{|v_{ij} \times p_i||v_{ij} \times p'_j|} \epsilon_{pp}^\pi \tag{5}$$

where $p_i = \{p_{ix}, p_{iy}, p_{iz}\}$ are a set of local unit vectors defined as $p_{ix} = p_{iy} \times p_{iz}$, $p_{iy} = (0, 1, 0)$ and $p_{iz} = \pi_i/|\pi_i|$. We employ the parameter set from [6] i.e. $\epsilon_s = -7.3\,eV$, $\epsilon_p = 0\,eV$, $\epsilon_{ss} = -4.3\,eV$, $\epsilon_{sp} = 4.98\,eV$, $\epsilon_{pp}^\sigma = 6.38\,eV$ and $\epsilon_{pp}^\pi = -2.66\,eV$.

III. ANALYTICAL EXPRESSION FOR LJ ENERGY ACROSS AN ABRUPT STEP

We consider an abrupt step of height h_0. The LJ energy is divided into three parts,

$$E_{LJ} = p_0 \sum_i \int_S \left(\frac{c_0}{|v_i - v'|}\right)^{12} - 2\left(\frac{c_0}{|v_i - v'|}\right)^{6} dv' = \sum_i E_{i,top} + E_{i,bot} + E_{i,sw}$$

where E_{sw} is due to the sidewall of the step of length h_0. We take the top edge of the sidewall as reference $(x, z) = (0, 0)$. A carbon atom located at $v_i = (x_i, z_i)$ will have the following energies,

$$\begin{aligned}
E_{i,top} &= \frac{\pi p_0 c_0^{12}}{1280(x_i^2+z_i^2)^{9/2} z_i^{10}} \left(128(x_i^2+z_i^2)^{9/2} + 315|x_i|z_i^8 + 840|x_i|^3 z_i^6 + 1008|x_i|^5 z_i^4 + 576|x_i|^7 z_i^2 + 128|x_i|^9\right) \\
&\quad - \frac{\pi p_0 c_0^6}{4(x_i^2+z_i^2)^{3/2} z_i^4} \left(2(x_i^2+z_i^2)^{3/2} + 3|x_i|z_i^2 + 2|x_i|^3\right) \qquad (6) \\
E_{i,bot} &= \frac{\pi p_0 c_0^{12}}{1280(x_i^2+\hat{z}_i^2)^{9/2} \hat{z}_i^{10}} \left(128(x_i^2+\hat{z}_i^2)^{9/2} + 315|x_i|\hat{z}_i^8 + 840|x_i|^3 \hat{z}_i^6 + 1008|x_i|^5 \hat{z}_i^4 + 576|x_i|^7 \hat{z}_i^2 + 128|x_i|^9\right) \\
&\quad - \frac{\pi p_0 c_0^6}{4(x_i^2+\hat{z}_i^2)^{3/2} \hat{z}_i^4} \left(2(x_i^2+\hat{z}_i^2)^{3/2} + 3|x_i|\hat{z}_i^2 + 2|x_i|^3\right) \qquad (7) \\
E_{i,sw} &= -\frac{\pi p_0 c_0^{12}(\hat{z}_i^2+x_i^2)^{9/2}}{1280(z_i^2+x_i^2)^{9/2} x_i^{10} (\hat{z}_i^2+x_i^2)^{9/2}} \left(315 z_i x_i^8 + 840 z_i^3 x_i^6 + 1008 z_i^5 x_i^4 + 576 z_i^7 x_i^2 + 128 z_i^9\right) \\
&\quad + \frac{\pi p_0 c_0^{12}(z_i^2+x_i^2)^{9/2}}{1280(z_i^2+x_i^2)^{9/2} x_i^{10} (\hat{z}_i^2+x_i^2)^{9/2}} \left(315 \hat{z}_i x_i^8 + 840 \hat{z}_i^3 x_i^6 + 1008 \hat{z}_i^5 x_i^4 + 576 \hat{z}_i^7 x_i^2 + 128 \hat{z}_i^9\right) \\
&\quad - \frac{\pi p_0 c_0^6}{4(z_i^2+x_i^2)^{3/2} x_i^4 (\hat{z}_i^2+x_i^2)^{3/2}} \left((z_i^2+x_i^2)^{3/2}(3\hat{z}_i x_i^2 + 2\hat{z}_i^3) - (\hat{z}_i^2+x_i^2)^{3/2}(3 z_i x_i^2 + 2 z_i^3)\right) \qquad (8)
\end{aligned}$$

where $\hat{z}_i \equiv z_i + h_0$. Note, carbon atoms where $x_i < 0$ will contributes to $E_{i,top}$ and $x_i > 0$ to $E_{i,bot}$ and $E_{i,sw}$. For $h_0 = 0$, the binding energy E_i reduces to,

$$E_i = \pi p_0 \left(\frac{c_0^{12}}{5 z_i^{10}} - \frac{c_0^6}{z_i^4}\right) \qquad (9)$$

which gives the expected z_i^4 scaling at large distance [4]. We compare our continuum model against the discrete version and obtains good agreement.

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