Overlaps in Stacked Graphene Flakes using Empirical Pseudopotentials

M. L. Van de Put*, W. G. Vandenberghe†, and M. V. Fischetti†
*imec, Kapeldreef 75, 3001 Heverlee, Belgium
*Condensed Matter Theory, Universiteit Antwerpen, Antwerpen, Belgium
†Dept. of Material Sciences, University of Texas at Dallas, Texas, USA
e-mail: vandeput.maarten@gmail.com

INTRODUCTION

Recently, resonant tunneling has been observed in stacked graphene flakes[1]. The rotational misalignment introduces an offset between the Dirac-cones in both flakes, resulting in negative differential resistance when shifting the Dirac-cones under bias.

In this paper we investigate the finite-size effect in nano-scaled graphene flakes. Improving on the bulk description, and because the structures are – atomistically speaking – large in size, we use the empirical pseudopotential method[2].

COMPUTATIONAL METHOD

To calculate the electronic states, we implement a local plane-wave empirical-pseudopotential eigenvaluesolver for large structures. We adopt the real-space technique used by Kresse and Furthmüller to solve the Schrödinger equations[3] in our problem. Using this method, we evaluate the kinetic energy in reciprocal space and the potential energy in real space. Using a diagonal operator in both spaces effectively reduces the complexity from a full rank matrix product with complexity $\mathcal{O}(n^2)$ to that of an FFT with complexity $\mathcal{O}(n \log n)$. Our eigensolver implements the Residual Minimization Method by Direct Inversion of the Iterative Subspace (RMMDIIS) first developed by by Wood and Zunger[4] and later used by Kresse and Furthmüller[3]. We selected this method because it allows semi-independent solution of the eigenvectors in parallel. This alleviates the lack of parallel computation on a k-grid, which is lacking in our closed systems.

To calculate the current, we make an approximation based on the Fermi-Golden rule. The current at a bias equal to $E_k^{\mathrm{T}} - E_{k'}^{\mathrm{B}}$ reads,

$$J = -2\pi \mathrm{e}\hbar^{-1}(E_i^{\mathrm{T}} - E_j^{\mathrm{B}}) \sum_{ij} \left[f^{\mathrm{T}}(E_i^{\mathrm{B}}) - f^{\mathrm{B}}(E_j^{\mathrm{T}}) \right] |\langle i, \mathrm{T}|\, j, \mathrm{B}\rangle|^2 ,$$

with $f^{\mathrm{T,B}}(E_k^{\mathrm{T,B}})$ the respective top and bottom Fermi levels determined by (electrostatic) doping, $\langle i, \mathrm{T}|\, j, \mathrm{B}\rangle$ the overlap between the top and bottom eigenstates with their respective energies E_i^{T} and E_j^{B}. This approximation assumes that electrons are always instantaneously refilled to their equilibrium states. For the current at finite temperatures we broaden the overlap using a thermal Gaussian.

RESULTS & DISCUSSION

Following the setup in Ref. [1] we have opted for a stacked structure as depicted in Fig. 1 A finite-length armchair-edged ribbon is placed on a ribbon with a zigzag edge with an angle close to $90°$. Note that we have not considered an intermediate layer and separated the layers 2 Å by vacuum.

The wavefunction of the first conduction states of the flakes is plotted in Fig. 2. As an example, we show their overlap as a function of rotation in Fig. 3. The Fermi-level of the layers is taken at 0.1 eV above the highest valence state for the armchair ribbon and 0.1 eV below the highest valence state for the zigzag ribbon, simulating doping. We show the resulting IV curve in Fig. 4 for different rotations. We observe that as we rotate the structure away from the $90°$ axis more resonance occurs as is evidenced by the NDR in the IV curves.

ACKNOWLEDGMENTS

I would like to acknowledge my promotors Wim Magnus and Bart Sorée for supporting my visit to the University of Texas at Dallas.

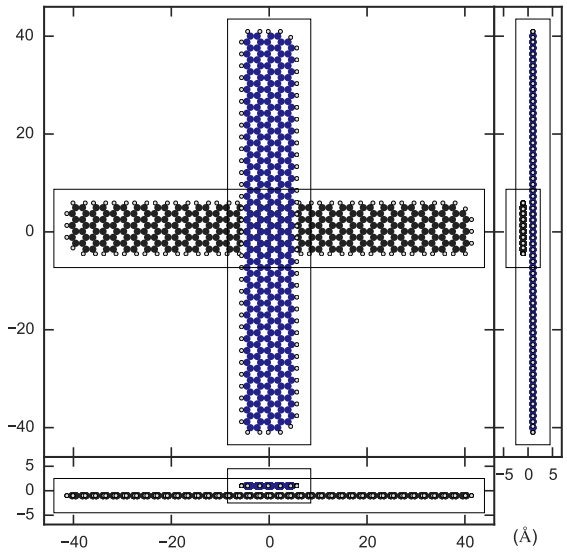

Fig. 1. The simulated structure. An armchair ribbon (horizontal) and a perpendicular zigzag ribbon (vertical). The bounding boxes show the supercell used.

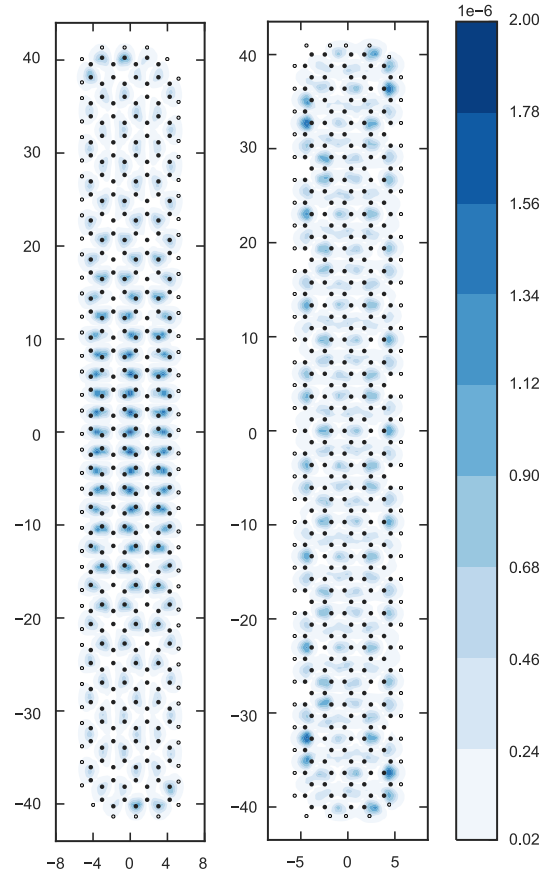

Fig. 2. The absolute squared wavefunction averaged along z of the first conduction states of the armchair (left) and zigzag (right) ribbons. Atom positions are shown for reference

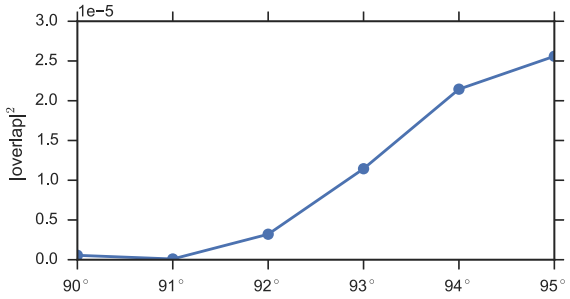

Fig. 3. The overlap of the first conduction states of the zigzag and armchair ribbons (shown in Fig. 2) at different rotations

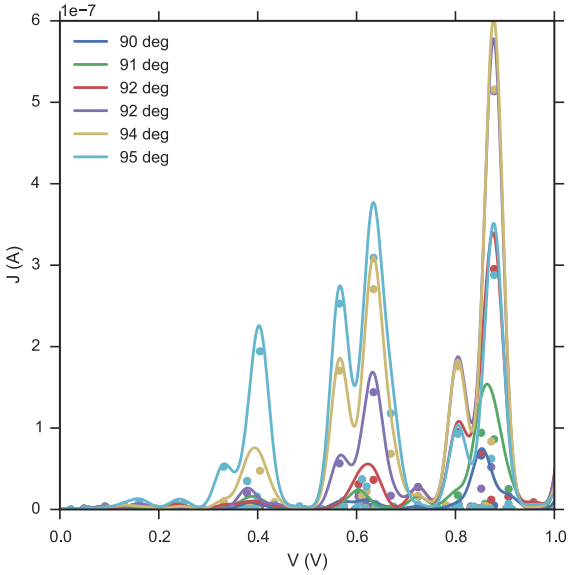

Fig. 4. The IV curve for different rotations. Zero temperature current is shown by discrete markers, for finite temperature 300 K the current is shown as a full line.

References

[1] A Mishchenko, JS Tu, Y Cao, RV Gorbachev, JR Wallbank, MT Greenaway, VE Morozov, SV Morozov, MJ Zhu, SL Wong, et al. Twist-controlled resonant tunnelling in graphene/boron nitride/graphene heterostructures. *Nature nanotechnology*, 9(10):808–813, 2014.

[2] Massimo V Fischetti and Sudarshan Narayanan. An empirical pseudopotential approach to surface and line-edge roughness scattering in nanostructures: Application to si thin films and nanowires and to graphene nanoribbons. *Journal of Applied Physics*, 110(8):083713, 2011.

[3] G. Kresse and J. Furthmüller. Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set. *Phys. Rev. B*, 54:11169–11186, Oct 1996.

[4] D M Wood and A Zunger. A new method for diagonalising large matrices. *Journal of Physics A: Mathematical and General*, 18(9):1343, 1985.