Towards an accurate tight-binding model of graphene under strain

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In this work, the effect of strain on the electronic structure of graphene modeled by several single-orbital third-nearest-neighbors tight-binding models is revisited. First, the Hasewaga et. al. [1,2] conditions for gap opening in uniformly strained graphene are revised to include up to third-nearest-neighbor interactions using parameters available in the literature. Briefly, the Hasewaga conditions set the limits before the Dirac cones merge, creating a gap. However this depends very much on the model used to compute the electronic structure. The typical model is the exponential decay with distance[2]. A comparison with ab-initio DFT calculations shows discrepancies for realistic uniaxial strain. DFT calculations indicate that the gap values and minimal strain to open gaps are very different. Based on the projection of the Kohn-Sham wavefunctions into localized orbitals, the disagreement is explained by an angular dependence of the second and third-nearest-neighbors tight-binding parameters (Figure 1).
We also propose that using the same distance dependent model, but with effective strain and lattice parameters, the DFT results of Figure 2 can be reproduced. This provides a consistent approach to modeling graphene under strain, combining the standard third nearest neighbor model which successfully reproduces the band structure in the whole Brillouin zone with a minimal distance dependence function, and a good description for the strain [3].

References

[1] Hasegawa, Y.; Konno, R.; Nakano, H.; Kohmoto, M., Phys. Rev. B. 74 (2006) 033413
[2] Pereira, V. M.; Castro Neto, A. H.; Peres, Phys. Rev. B, 80 (2009) 045401
[3] Botello-Méndez, Obeso and García Naumis (submitted).

Figures

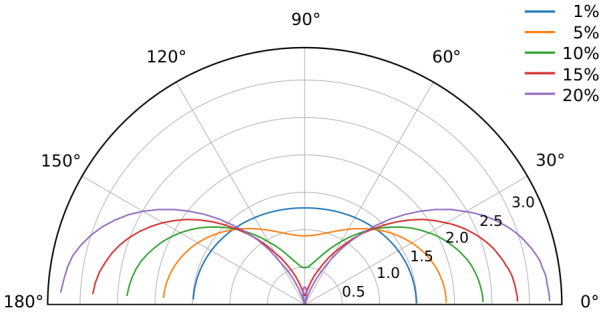

Figure 1: Dependence of the second nearest neighbor hopping parameter with strain direction with respect to the zigzag direction for different values of strain.

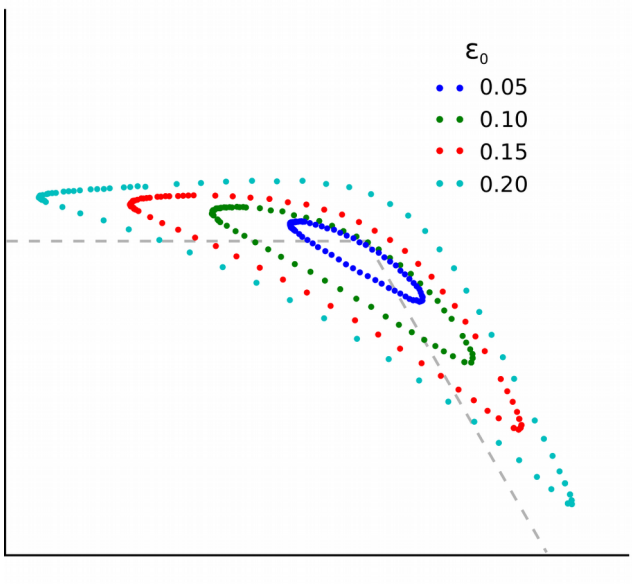

Figure 2: Position of the Dirac cone as a function of strain magnitude and direction