Ab initio quantum transport in polycrystalline graphene

Samuel Dechamps, Viet-Hung Nguyen, Aurélien Lherbier, and Jean-Christophe Charlier

Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, 1348 Louvain-la-Neuve, Belgium.

samuel.dechamps@uclouvain.be

Out of the different production approaches for two-dimensional materials such as graphene, chemical vapor deposition (CVD) is presently by far the most viable and industry compatible one. However, CVD materials are found to be polycrystalline in nature and composed of many single-crystal domains separated by grain boundaries (GBs) of irregular shape, made up by pentagons, hexagons and heptagons, as depicted in Fig.1. The structural defects forming those GBs strongly affect the overall properties of wafer-scale graphene [1]. Additionally, GBs are an important source of scattering that limit drastically the carrier mobility and consequently the performance of graphene-based electronic devices. Only a few *ab initio* studies have been performed so far on GBs, mostly with ideal geometries. In the present research, highly-efficient simulations based on density functional theory have been used to explore both charge and spin transport in polycrystalline graphene, including spin-orbit couping via non-collinearity.

Firstly, charge and spin transport properties are investigated for simple GB geometries exhibiting two different electronic structures, as formerly described in the literature [2].

Secondly, charge transport properties are also predicted *ab initio* for more complex but highly realistic GB geometries, including thousands of atoms (as illustrated in Fig.1).

Simultaneously, the effect of out-of-plane corrugation on both charge and spin transport is analysed for localized buckling in pristine graphene. At last, both effects of corrugation and the presence of structural defects in GBs are scrutinized for various buckling heights.

In summary, the goal of the present research intends to contribute to a more comprehensive understanding at the atomistic level of the possible detrimental effect of GBs on the electronic transport in polycrystalline graphene by considering various realistic case studies.

References

[1] P.Y. Huang, et al., Nature 469, 389-392 (2011)

[2] O.V. Yazyev and S.G. Louie, Nat. Mater. 9, 806–809 (2010)

[3] S. Dechamps, V.-H. Nguyen, A. Lherbier, and J.-C. Charlier, in preparation (2016).

Figures

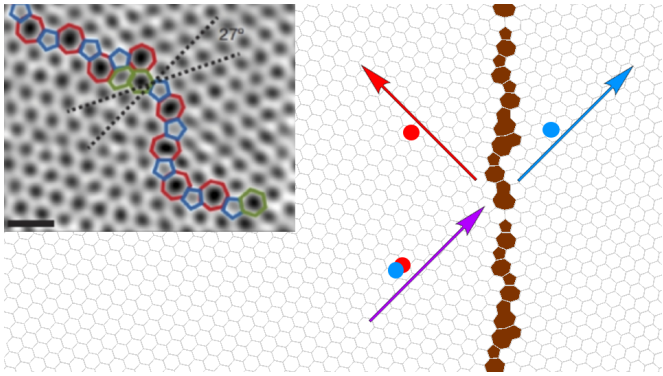

Figure 1. Modeling electronic transport through grain boundaries in polycrystalline graphene. High-resolution TEM image (from Ref[1]) of a grain boundary compared with an atomistic model, based on hexagons, heptagons and pentagons. Colored arrows illustrate both the reflexion and the transmission of travelling electrons with different spin states throughout a realistic grain boundary in graphene.