Discussion summary: Strain in graphene

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(Dated: July 30, 2009)

After the tutorial conducted by A. Mirlin on the Non Linear σ-model, a discussion centred on the effects of strain in graphene begun, motivated by the morning session on Raman spectroscopy. The discussion was opened by M. Fogler suggesting that a strain of 20 % used in the Tight Binding (TB) approach presented by N. Peres (Phys Rev. B **80** 045401) may be too large compared to what conventional materials can resist, usually no more than a few percents. Following the arguments of his morning talk, N. Peres exposed that certain experiments (K.S. Kim *et al.* Nature **457** 706) which sandwich graphene between two substrates are able to produce a substrate strain of 18 %. The experimental measure of the anisotropy in the resistivity produced by bending agrees with the TB calculation assuming graphene is strained as much as the substrate. He commented that the question that should be addressed is the applicability of the linear elasticity theory. He also stated that DFT calculations agree with the hopping parameters obtained within linear elasticity.

Regarding the validity of linear elasticity in this context, M. Katsnelson pointed out that given the Young modulus in graphene is $Y = 1$ TPa, and considering a strain of the order of 20% the energy per carbon atom is ~ 1 eV. He noted that the formation energy of vacancies is higher, near 7 eV, and the one for dislocations, although not yet known, can be of the same order. Moreover, he commented that in his simulations he did not observe any defects even at high temperatures (~ 3500 K). He remarked the importance of evaluating the applicability of linear elasticity theory and of the related issue of the formation of dislocations.

Regarding what N. Peres stated, A. Ferrari argued that it is difficult to get strains over few percent, and that the stress applied to the substrates in the Nature paper do not necessarily translate to the corresponding strain for graphene. N. Peres agreed with this point, and suggested that compression could be a much more effective way of inducing high strains. A. Ferrari also pointed out that it should not be difficult to decide how much strain is being transfered to graphene by performing a Raman measure during the bending process, because a strain as large as 20% would produce dramatic changes in the Raman spectrum of graphene. Moreover, he also commented that in the Raman spectrum presented in the Nature paper it is not clear whether they actually have a monolayer or not, a comment with which N. Peres also agreed.

N. Peres then concluded that assuming that the experiment can be interpreted as having a monolayer with 20% strain, then the results of the TB calculation are in agreement with the resistivity measurements, although this may very well be a coincidence.

After that, a new topic was raised by Alina Veligura, who asked what would be the best type of graphite to obtain graphene: Kish graphite (with high mobility), Highly Orientated Pyrolitic Graphite (HOPG) or natural occurring graphite. The question was answered by A. Ferrari by stating that, although being an interesting question, no systematic work has been done to characterize the differences among graphene samples obtained from these three types of graphite.