CHARGE CARRIERS IN FEW LAYER GRAPHITE

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The recent transport measurements on monocrystalline graphite containing only few layers (few layers graphite or FLGs) have demonstrated the potential technological importance of pure graphitic materials in semiconductor applications. Indeed, the possibility of switching from electron to hole transport was demonstrated experimentally by Hall measurements. FLGs have also been shown to behave like mixed carriers semimetallic systems, with a domain of coexistence of electrons and holes [1]. However, the exact thickness and staking order of the graphitic thin film was not unambiguously determined.

Differently to the three dimensional graphite bulk structures, electrons in FLGs are confined along one crystallographic direction, offering a genuine 2D character of its electronic response. However, the linear dispersion of the electronic bands near the Fermi level that appears in monolayer graphene is lost, as a consequence of the interaction between layers. The resulting complex dispersion relations and overlap between electron and hole bands leads to the experimentally observed coexistence of different type of carriers. The experimental data indicate an overlap in the 4 to 20 meV range.

In the present communication we report the detailed investigation of the electronic structure of FLG with 2 to 4 layers by *ab-initio* technique (ABINIT code). The different energetically favoured possible stackings of FLG that we studied are : AB, ABA, ABC, ABAB, ABCA, ABAC (identical to ABCB) .

We have demonstrated how the number of layers and of the geometry-dependence of the interlayer interaction influence the nature of the charge carriers in FLGs. Indeed, amongst 3 and 4-layer films, ABAC is found to be a narrow gap semiconductor (Eg=8.8 meV) and is then exclude to be the experimentally grown morphology. The other stacking exhibit metallic behaviour with various characteristic : The rhombehedral family (ABC, ABCA) demonstrates or very small (< 3 meV) overlap between electrons and holes bands. The Bernal family (ABA, ABAB) presents overlaps in agreement with experimental observations (from 5 meV to meV)

In conclusion, we have shown that field effect behaviour of FLG observed by Novoselov et al. is intrinsic properties of the systems and that Bernal family ABA and ABAB stacking could explain the experimental data.

Further details on the present communication can be found in [2]

References:

[1] K.S. Novoselov et al., Science **306** (2004), 666.
[2] S. Latil, L. Henrard. Phys. Rev. Lett. Accepted (2006)