Frictional mechanisms in few-layer graphene

M.C. Righi[1], M. Reguzzoni[1,2], A. Fasolino[3], Mattia Sacchi[1,2], Elisa Molinari[1,2]

[1] Istituto Nanoscienze, CNR - Consiglio Nazionale delle Ricerche, I-41125 Modena, Italy
[2] Dept of Physics, Informatics and Mathematics, University of Modena & Reggio, I-41125 Modena, Italy
[3] Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 Nijmegen, NL

Corresponding author: mcrighi@unimore.it

In micro- and nano-scale applications the thickness of a solid lubricant represents a very important factor to preserve relevant interactions (e.g. magnetic) between the sliding materials. Graphene --a revolutionary material for its known electronic and mechanical properties— has great potential also in this context as the thinnest solid lubricant. The fundamental mechanisms governing friction are however not yet clear, and important issues are still open e.g. concerning the role of multiple graphene layers [1].

We investigate the friction mechanisms in multilayer graphene films by calculating the potential energy surfaces (PES) from first-principles [2], and by simulating the motion of a model tip on the films by classical molecular dynamics [1].

From the ab-initio PES we derive an analytical expression the describes the interaction energy between two graphene layers vs their relative position. Thanks to its formal simplicity, the proposed model allows for an immediate interpretation of the interlayer binding and the potential corrugation. The latter plays a crucial role in determining the intrinsic resistance to interlayer sliding and controls the frictional behaviour under load (fig. 1). We show that the dominant mechanism in these π-bonded systems is the increase in Pauli repulsion with load, while the effect of van der Waals adhesion is negligible.

To understand the role of N-layer graphene films, we evaluate both the PES modifications as a function of N [3] and the onset of mechanisms of energy dissipation due to interlayer motions during finite temperature simulations [1]. We find that a sliding tip on a supported few-layer film induces both out-of-plane (fig. 2) and in-plane deformations, which increase with the number of layers in the film. We elucidate a new frictional mechanism connected with shear layer motions.

[1] M. Reguzzoni, A. Fasolino, E. Molinari, M.C. Righi, J. Phys. Chem. C 16, 21104 (2012), and references therein.

[2] M. Reguzzoni, A. Fasolino, E. Molinari, M.C. Righi, Phys. Rev. B 86, 245424 (2012).

[3] M.C. Righi et al, to be published.

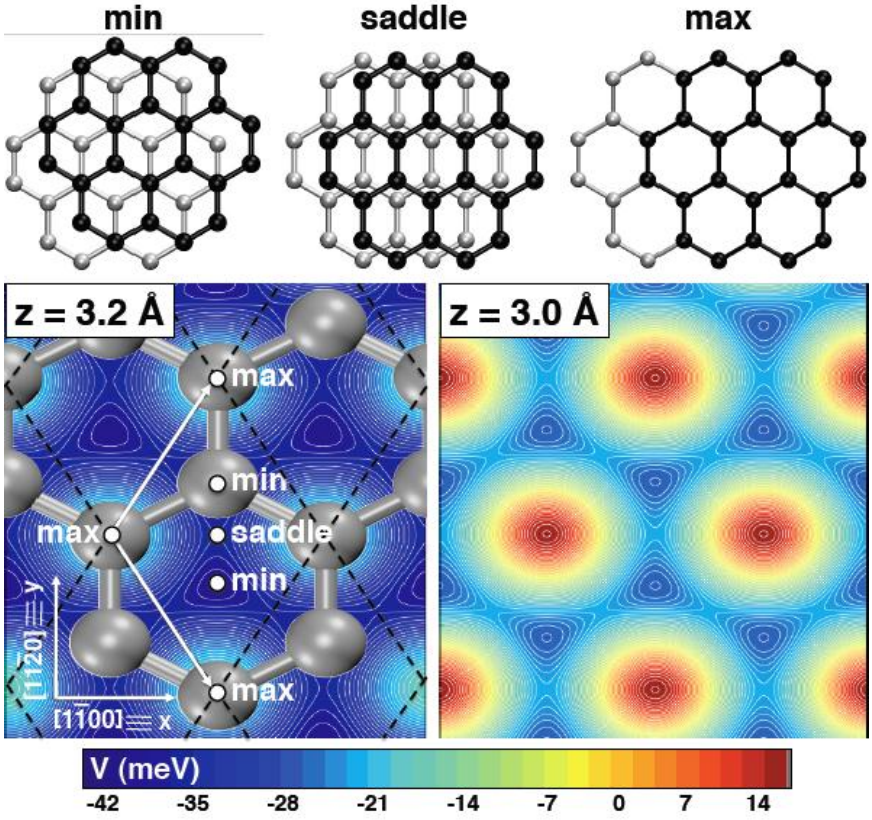

Fig. 1. PES function for bilayer graphene, represented in two dimensions for two different values of the interlayer separation *z*. The bilayer configurations corresponding to the PES stationary points are illustrated in the top part of the picture.

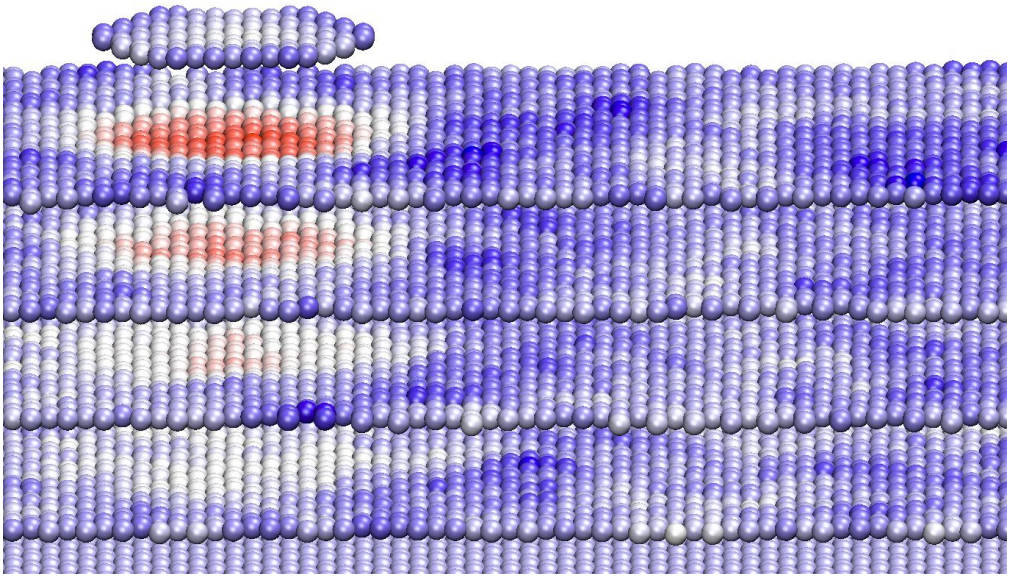

Fig. 2. Equilibrated structure of a 4-layer graphene film. The colour code indicates the deviation of the particle height from that of the layer center of mass. Blue corresponds to 0.4 Å and red to – 0.9 Å.