Ab initio and semi-empirical simulations of tip-sample interactions on Graphite(0001) surface

V. Caciuc, H. Hölscher and H. Fuchs
Physikalisches Institut, Westfälische Wilhelms Universität Münster, Germany
caciuc@uni-muenster.de

Graphite(0001) surface as substrate is a common choice in surface science due to lack of chemical reactivity. Therefore this surface was the subject of intensive experimental studies by means of scanning probe techniques such as Non-Contact Atomic Force Microscopy (NC-AFM). Atomic-scale contrast has been obtained for clean surface [1] as well as for single-walled carbon-nanotubes [2].

From structural point of view, the graphite(0001) surface consists of ABA stacking layers of carbon atoms with hexagonal coordination such that there are two non-equivalent carbon sites. The NC-AFM image [1] of this surface exhibits a trigonal pattern of maxima and minima. Counterintuitively, the simulated NC-AFM images obtained for a semi-empirical Lennard-Jones potential [3,4] showed that the maxima originate from the hollow sites while the two non-equivalent carbon atoms are visualized as two different minima.

The semi-empirical simulations of the NC-AFM images of graphite(0001) essentially relies on the assumption of different equilibrium distances of the AFM tip on top of the two inequivalent carbon atoms. We investigated the quantum mechanical origin of this assumption by performing *ab initio* simulations. Our simulations suggest that the tip-sample interactions at these carbon sites are indeed different and that this difference originates from a different relaxation pattern of the graphite(0001) surface. This conclusion is also supported by first-principles simulations of the interaction between an AFM tip and a graphene layer.

Even if for a single-walled carbon nanotube there is only *one* type of carbon atom, our semi-empirical simulations clearly show that in a NC-AFM image the hollow sites must appear as maxima and the carbon atoms as minima. This finding agrees well with the experiment [2,4].

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