Constant height AFM simulation of graphite substrate and flake

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Theoretical simulation of AFM(FFM) images for systems including not only surface and tip but also movable substances like flake or molecule on the substrate is significant to understand the mechanism of friction and lubrication reducing the quantitative gap between experimental data and simulation results [1][2]. Moreover, the approach reported here can be expanded to the simulation of AFM images for biological molecules without much difficulty. We report here a method and typical results of constant-height-AFM simulation of the graphite flake and the simple organic compound on the graphite substrate with or without vacancy on the surface. We also developed AFM motion draw tool which can visualize how each atom moves at each step of simulation. It helps to understand the atomistic processes during the tip scan intuitively.

We used the same potential model and calculation method as the simulation of only tip and substrate performed before [3]. Model (a): Flake is on the substrate and tip scans above the flake. Force image shows only the substrate atoms when the scan distance is relatively close to the flake, while the flake atoms can also be seen in the image when the tip is relatively far from the flake. Image of motion shown at the same time with the force image clearly tells us that the flake skip from one meta-stable position to another in former case, while the flake can not skip over potential barrier in later case, so it just moves back and forth.
Model (b): Small flake in the vacancy is scanned. Resulting image is in the right plane of Fig. 1. Atomic resolution can not be obtained for flake itself unlike substrate atoms surrounding the flake. Motion image again clearly shows that it is because the flake rotates while the tip passes above the flake.

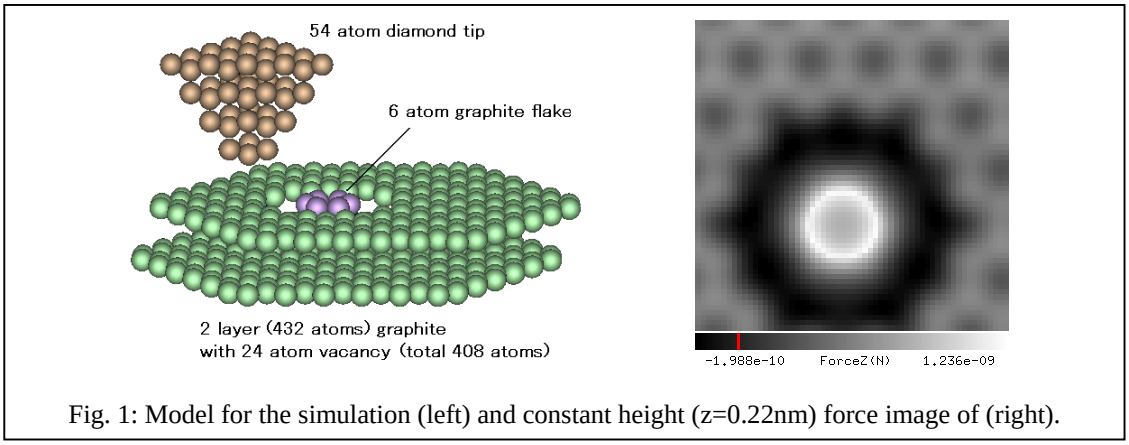

Fig. 1: Model for the simulation (left) and constant height (z=0.22nm) force image of (right).

[1] N. Sasaki, K. Kobayashi, and M. Tsukada, Phys. Rev.B 54, 2138 (1996)
[2] N. Sasaki, M. Tsukada, et al. Phys. Rev.B 57, 3785 (1998)
[3] N Sasaki, M. Tsukada, Phys. Rev.B 52, 8471 (1995)