Modelling of dynamic AFM imaging of alkanethiols on Au (111)

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Self-assembled monolayers of long-chain molecules is a promising class of systems with widespread potential applications in materials science. For example, SAMs can be used as a template for molecular imaging and for production of high-precision patterns with different methods, in particular, Atomic Force Microscopy (AFM).
We have modelled the structure of self-assembled monolayers of decanethiols [$S(CH_2)_9CH_3$] on atomically flat and rough gold surfaces using the united-atom semi-empirical approach. The potentials developed by Hautman and Klein [1] with the interaction of the CH_3, CH_2, and S particles with Au atoms fitted by Tupper and Brenner [2] were adopted. The behaviour of the system has been studied when local orientational defects and cavities are introduced into the system. Lower-coverage phases have been optimized to obtain clusters of alkanethiol molecules on gold and to model the behaviour of the monolayer on substrate terraces. Full-coverage structures have been optimized on steps and terraces on the gold substrate to simulate SAMs on rough gold surface. Non-Contact Atomic Force Microscopy (NC-AFM) images of the optimized configurations were modelled. The resolution of the AFM images of the monolayers obtained with gold tip, with CH_3 modified gold tips as well as with SiO_2 tips will be discussed.
This study will help to understand different conformations of monolayers of alkanethiols on Au (111) in different experimental conditions as well as to find the optimum tip material for high resolution NC-AFM of these systems.

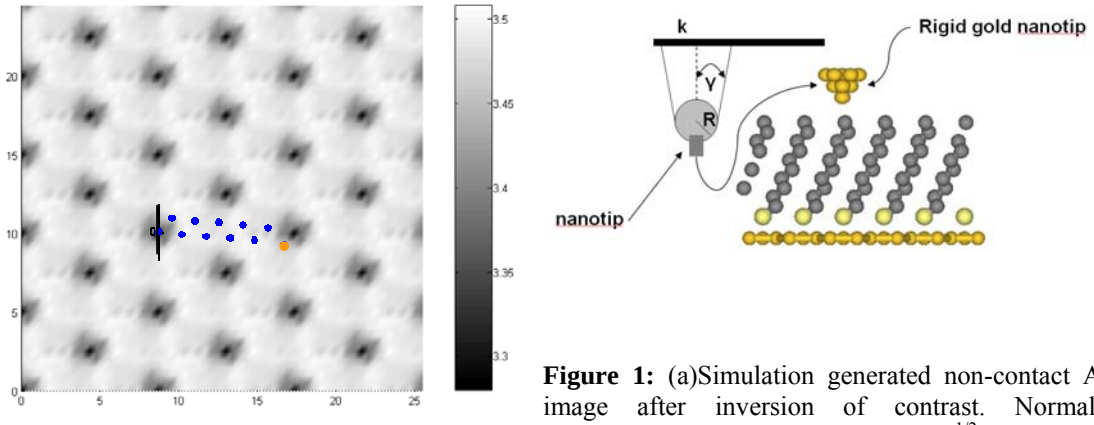

Figure 1: (a)Simulation generated non-contact AFM image after inversion of contrast. Normalized Frequency Shift $\Delta f = 0.0440$ fN x $m^{1/2}$. The blue and yellow balls specify the initial position of one of the molecules. The blue ball with the line is the CH_3 group, the blue balls are the CH_2 groups and the orange is the Sulphur group. The dark spots correspond to CH_3 sites. (b) SAMs with the Au tip. The tip consists of a macroscopic part (cone with a sphere at the end) and a 9 atom pyramidal rigid gold nanotip.

[1] J. Hautman, M.L. Klein, J. Chem. Phys. 91 (8), 1989, 4994-5001
[2] K.J. Tupper, D.W. Brenner, Langmuir 1994, 10, 2335-2338