Investigating conservative and non-conservative tip-surface interactions with the Virtual Atomic Force Microscope

T. Trevethan[1], **L. Kantorovich**[1], J. Polesel-Maris[2], S. Gauthier[2]
[1]Department of Physics, Kings College London, Strand, London WC2R 2LS, UK
[2]CNRS, CEMES, 29 Rue Jeanne Marvig, F-31055 Toulouse 4, France
thomas.trevethan@kcl.ac.uk

It has long been a challenge in interpreting the results of NC-AFM experiments to separate out the physical effects due to the tip-surface interaction from the complex motion of the oscillating cantilever and finite response of the instrumentation and electronics controlling the device. In order to try and better understand this interplay, a virtual machine has been created [1] to model numerically the operation of the entire experimental apparatus with a tip-surface interaction that was calculated from realistic modelling.

In this presentation, we describe recent results obtained with the Virtual AFM, in which both conservative and non-conservative interactions between the tip and surface were incorporated using the theory of dynamical response at close approach in scanning probe microscopy [2]. These results show conclusively that the damping signal contrast observed in atomic resolution NC-AFM experiments is due to dissipative interactions in the tip-surface junction due to adhesion hysteresis effects and not an artifact of the apparatus. We performed scans of the MgO (001) surface with a MgO tip that show the same contrast patterns and magnitude of dissipated energy as previous calculations using a sinusoidal approximation for the tip oscillation trajectory that do not take into account the effect of electronics. Using a simple model for the energy states and barriers for atomic processes on the surface, we show how the topography and damping images depend on the various experimental parameters, such as lateral velocity, set amplitude and frequency points and the extent of thermal noise.

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