

General Theory of NC-AFM at a Close Approach: from Imaging to Dissipation

Lev Kantorovich and Tom Trevethan

Physics Department, King's College London, London, WC2R 2LS, U. K

It is well known that atomic resolution in the NC-AFM imaging becomes only possible if during experiment the tip comes very close (one-two atomic distances) to the surface. At such experimental conditions dissipation effects become significant as well, and also demonstrate atomic resolution. Using Molecular Dynamics (MD) simulations, we have proven recently that the main mechanism responsible for the atomic-scale dissipation in the NC-AFM experiments originates from atomic instabilities. These appear when atoms in the junction experience a superposition of the potential energy surfaces of the tip and surface at close approach. At the same time, existence of such instabilities should result in strong dependence of atomistic processes during the scan, and thus both topological and dissipation (damping) images, on temperature.

Theories of the NC-AFM available so far are based on the existence of a single potential energy minimum for the system in the junction and thus do not allow for atomic instabilities (such as e.g. atomic jumps between the two surfaces). Consequently, these theories do only work at zero temperature.

We present a general theory of the NC-AFM which lifts all mentioned above limitations. The theory enables one to calculate, on the same footing, both the frequency shift and the excitation signal amplitude for the tip oscillations in the conditions of close approach when atomic instabilities are most likely to occur. In our theory the force acting on the tip is time dependent and thus naturally differs on approach and retraction. The calculation of the required potential energy surfaces at each tip position can be done using available zero temperature total energy tools (either *ab initio* or semiclassical). We demonstrate that atomic instabilities result in jumps in the frequency shift and, at the same time, sharp increase in atomic scale dissipation. Both effects show a pronounced temperature dependence.

The general theory is illustrated on a simple reference system in which a cube MgO tip is used to scan the MgO (001) surface, and the interaction between atoms is modelled by a semiclassical force field using our home-made Sci-Fi code specifically designed for the NC-AFM studies. The calculated dissipation energies show atomic scale dissipation and are of the order of an eV.