SIMULATIONS OF CONTROLLED SINGLE ATOM MANIPULATION IN NON-CONTACT ATOMIC FORCE MICROSCOPY

T. Trevethan[1], M. Watkins[1], L.N. Kantorovich[2] and A.L. Shluger[1]
[1]Department of Physics and Astronomy, University College London, London, UK
[2]Department of Physics, Kings College London, London, UK
t.trevethan@ucl.ac.uk

One of the great achievements of scanning probe microscopy is the controlled manipulation of individual atoms on surfaces. Non-contact atomic force microscopy (NC-AFM) is the only tool capable of imaging and now manipulating individual atoms of the surfaces of insulating materials [1]. We present the results of calculations performed to model the process of manipulation using two model but technologically important systems: an oxygen vacancy and a metal adatom on the regular MgO (001) surface. The accessible states of the systems and the barriers that separate them are determined as a function of tip height and position above the surface from atomistic calculations. The dynamical evolution of the system in real time as the tip is oscillated and at a finite temperature is then determined using a Kinetic Monte Carlo method. It is found that the point at which the manipulation occurs is sensitive to both the temperature and the trajectory of the cantilever. Based on the results of these calculations we are able to identify the most favourable experimental conditions and the procedure to achieve the desired manipulation.

We show how the manipulation occurs as a single atomic scale event, which results in a large and sudden change in the force-field experienced by the tip during a single oscillation cycle. Using a Virtual dynamic atomic force microscope [2], which explicitly simulates the operation and response of the real apparatus, we show how this single atomic scale event can be registered by the instrument and used as an experimental signal that the manipulation has been achieved.

References:

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