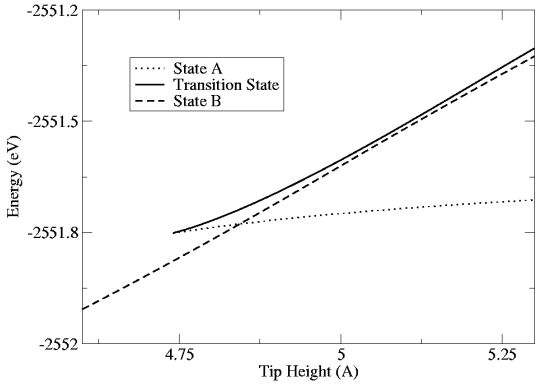
Atomic scale contrast in damping images of ionic surfaces

T. Trevethan, L. Kantorovich
Department of Physics, Kings College London, Strand, London WC2R 2LS, UK
thomas.trevethan@kcl.ac.uk

It has become apparent in recent years that the most likely cause of atomic scale contrast in damping images obtained in Non-Contact Atomic Force Microscopy (NC-AFM) experiments is a non-conservative tip-surface interaction due to adhesion hysteresis in the tip-surface junction at close approach, involving significant displacement of a single atom in either the surface or tip [1,2]. In this submission we present the results of extensive atomistic modelling of the tip-surface junction for a number of model systems, including the MgO, CaO and NaCl (001) surfaces with a MgO tip. The various accessible states and transition barriers of these systems are calculated as a function of tip position above the surface, leading to a complete description of the accessible energy landscape, as apposed to the single local minimum usually considered in NC-AFM modelling. An example of this is illustrated in the figure below which shows energy states as a function of vertical tip position above the surface for an Mg terminated MgO tip above a Cl atom in the NaCl (001) surface. Using this data with the transition state theory of dynamical response in NC-AFM [3], we produce topography and damping images of the three ionic systems with both tip terminations that show several contrast patterns that depend on the frequency shift set point and temperature of the system.

The reversibility of the tip-surface atomic jumps with tip retraction is discussed in relation to the system temperature and the tip vertical velocity, which has implications for image stability and atomic manipulation. The strong dependence of the contrast on the exact nature of tip apex is discussed in detail. We also explain how the tip apex polarity and surface sub-lattice can be determined from the combination of topography and dissipation images.



[1] T. Trevethan, L. Kantorovich, Nanotechnology **16**, S79 (2005)
[2] S. Hembacher, F. J. Giessibl, J. Mannhart, C. F. Quate, Phys. Rev. Lett. **94**, 056101 (2005)
[3] L. N. Kantorovich, T. Trevethan, Phys. Rev. Lett. **93**, 236102 (2004)