Measured vs. computed force-distance curves on NaCl(001)

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Species leading to maxima in non-contact AFM images of ionic crystal surfaces can be identified via comparison with atomistic simulations based on shell model potentials and plausible models for the tip apex [1]. The required comparison relies on characteristic changes in images recorded at different distances or frequency setpoints [2] or on force vs. distance curves extracted at judiciously chosen sites [3]. As recently demonstrated for KBr(001) [3], sublattice identification is possible even when surface unit cell is highly symmetric and contains no inequivalent sites with the same species. These images or force curves must be obtained in a range where no discontinuities due to atom jumps occur [4].

Using the same low temperature instrument [5] and measurement protocol, undistorted atomically resolved non-contact images were previously obtained on a NaCl(001) sample cleaved and heated in UHV. Resonance frequency vs. distance data were recorded above maxima and minima in the images and converted to force data. These data are compared with computed short-range forces after subtracting a sum of site-independent Van der Waals and electrostatic contributions which provide an excellent fit between 12 and 0.5 nm. Alternatively, the difference between forces obtained above the maximum and the minimum is compared directly. In either case semi-quantitative agreement is achieved with computations which assumed a Na^+ terminated NaCl tip.

Computations have been performed for an oxidized tip or one which sample material picked up, represented by a MgO or a NaCl cubic cluster, respectively. As in the case of KBr(001) [3], computed forces exhibit no jumps if the tip consists of the same material as the sample, even at distances below the force minimum. However, in accordance with earlier simulations on LiF(001) [1], irreversible ion hops occur to the MgO tip before the force minimum is reached, owing to a stronger attraction to the closest sample ions. As a result, a chain of sample ions with alternating signs is pulled out upon retraction. In the present relaxation simulations, the ions come back into their original positions upon reapproach, almost following the reverse sequence. However, a long enough chain is expected to break once thermal agitation is included, and to collapse into a cluster at the tip apex.

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