

Microscopic Insights into atomically resolved Contact Potential Variations

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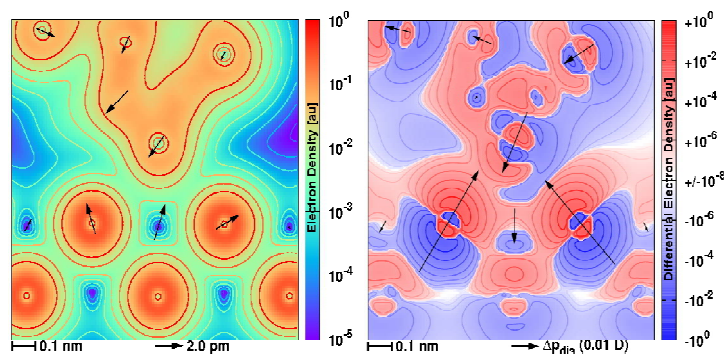
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We present a multiscale model of the atomistic-scale variations of the local contact potential difference (LCPD) revealed by Kelvin probe force microscopy (KPFM) on surfaces of ionic crystals. In a first step, the electrostatics of the macroscopic tip-cantilever-sample system is treated by a finite-difference method on an adjustable non-uniform mesh. Results are compared with the solution for a conducting sphere against a thick dielectric slab [1]. Owing to the significant electric field penetration into the dielectric, the tip shank and the cantilever also affect that force and its gradient, even at sub-nanometer tip-surface separations where atomic-scale contrast appears. The applied bias affects the electrostatic forces in the atomic scale on the surface through the electric field under the tip-apex which is inserted, as the second step, into a series of *ab initio* computations. This yields bias-dependent forces on atoms as well as the induced changes in electronic density and displacements of the ions in response to the bias. Expressions for amplitude modulation (AM) and frequency modulation (FM) Kelvin signals and for the corresponding local contact potential differences (LCPD) are obtained by combining the macroscopic and atomistic contributions to the force component generated at the voltage modulation frequency. Then by averaging over an oscillation cycle, the KPFM signal is evaluated for several amplitudes [2].

As an alternative to evaluate the LCPD with no need to have the force-bias parabola, we present a microscopic theory for the atomic-scale variations of the LCPD by splitting the electrostatic interaction into contributions according to their linear or quadratic dependence on the bias voltage. This way analytic expressions for the KPFM signal and approximations are obtained for intermediate- and short-range contributions in terms of the dipole moment and polarizability of the subsystem, and of induced changes in the electron density and ionic displacements, respectively. The distance dependence of the LCPD contrast is shown to mirror the dependence of the perpendicular dipole moment when the long-range, site-independent LCPD is compensated. Results are illustrated for a realistic silicon nano-scale tip interacting with a NaCl(001) sample treated by density functional theory.

Figure: Total and differential electronic density of a model Si-tip separated by 0.32nm from NaCl(001) surface in response to applying a unit bias on a macroscopic model probe. The arrows show either the ionic displacements from the protosystem due to chemical interactions or the induced ionic dipole moments in response to the electric field.



References

- [1] A. Sadeghi, A. Baratoff and S. Goedecker, submitted abstract
- [2] A. Sadeghi, A. Baratoff, S. A. Ghasemi, S. Goedecker, A. Baratoff, T. Glatzel, S. Kawai, E. Meyer, to be published.