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Multi-Scale Approach to Simulations of Kelvin Probe Force Microscopy[1] ALI SADEGHI, ALIREZA GHASEMI, STEFAN GOEDECKER, ALEXIS BARATOFF, THILO GLATZEL, ERNST MEYER, University of Basel — The distance dependence and atomic-scale contrast recently observed in nominal contact potential difference(CPD) signals simultaneously recorded during noncontact atomic force microscopy on surfaces of insulating and semiconducting samples have stimulated theoretical attempts to explain how the applied bias voltage affects electrostatic forces acting on the atomic scale. We attack the problem in two steps. First, the electrostatics of the macroscopic tip-cantilever-sample system is treated by a finite-difference method on an adjustable nonuniform mesh. It has the advantages of getting a systematically increasable accuracy as well as the ability of considering the cantilever which turns out to be important for insulating samples. The resulting electric field near the tip apex is then inserted into a series of wavelet-based density functional theory calculations. Results are obtained for a reactive disordered neutral silicon nano-scale tip interacting with a NaCl(001) sample. Bias-dependent forces and resulting atomic displacements are computed to an accuracy of 1 pN. Theoretical expressions for Kelvin signals and local contact potential difference (LCPD) are obtained combining both contributions to the electrostatic force and evaluated for several tip oscillation amplitudes.

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