# Consequences of multi-scale theory of Kelvin Force Microscopy with atomic resolution

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The distance dependence and atomic-scale contrast observed in nominal contact potential difference (CPD) values simultaneously recorded with non-contact atomic force microscopy (NCAFM) have stimulated theoretical attempts to explain such effects. Especially in the case of insulators, the local CPD (LCPD) is not an intrinsic property, and it is not clear how the applied bias voltage affects electrostatic forces varying on the atomic scale. We attack the problem via coupled macroscopic and microscopic computations described at previous NCAFM Conferences and elsewhere [1]. Details and an improved treatment of the microscopic problem are described in a separate contribution [2]. Here we focus on consequences for AM and FM-KPFM measurements on defect-free surfaces. Compared to a conducting sample, due to field penetration into an insulator, the electrostatic force on the macroscopic probe (tip plus cantilever) is reduced and more strongly influenced by the cantilever and the tip shank, while the force gradient is affected by the latter. At separations much smaller than the tip radius, both quantities, as well as the electric field in the vacuum gap are enhanced, albeit much less than for a conductor. Over a few nanometers this macroscopic field is essentially uniform and is applied to the microscopic subsystem (tip apex represented by a cluster plus a wider slab of a few layers of the sample). Results are illustrated for a reactive Si tip above NaCl(001), but most of our conclusions are general.

The site-dependent part of the LCPD (defined as the DC bias which nulls the Kelvin signal) is given by the slope $dF_\mu/dV$ of the microscopic force divided by the curvature $d^2F/dV^2$ of the force versus bias. Both quantities are averaged over the tip oscillation with different weights in AM and FM KPFM, and their dependences on the amplitude $A$ are elucidated (see the Figure). The atomic-scale LCPD contrast is predicted to be stronger in the FM mode, e.g. by a factor ~ 10 for typical $A$ = 5 to 20 nm in our example. This prediction is consistent with experimental data obtained Si(111) 7x7 samples with sputtered Si tips [3,4]. Because $d^2F/dV^2$ is dominated by the macroscopic electrostatic force, it is desirable to extract the more fundamental quantity $dF_\mu/dV$. Possible procedures might be discussed.

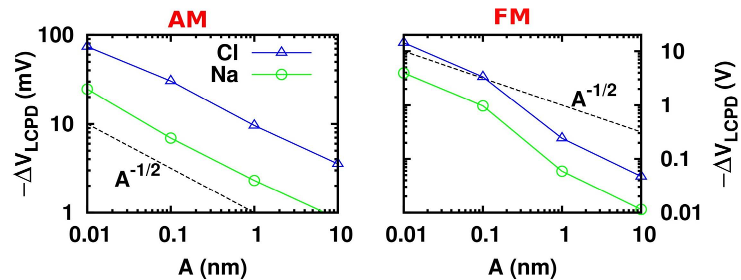


*Figure: Predicted amplitude dependence of the site-dependent LCPD in AM and FM KPFM for a reactive Si tip 0.3nm away from a NaCl(001) sample. The distance dependencies are the same in both modes if A > 0.1 nm, but the amplitude dependence remains the same[2].*

## References

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[2] A. Sadeghi, A. Baratoff and S. Goedecker, submitted abstract
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