Unambiguous Interpretation of Atomically Resolved Force Microscopy Images of an Insulator

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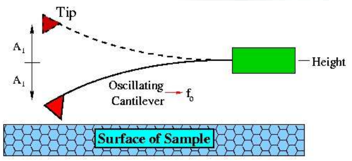
Introduction

Atomic resolution has now been achieved on several insulating and semi−conducting surfaces using Non−contact Atomic Force Microscopy (NC−AFM). However, in most cases, due to the high symmetry of the lattice, the identity of atomic sized features is impossible to establish . Further progress requires characterization of the tip on the atomic scale and better understanding of the tip−surface interaction. One possible approach to this problem is by combining theoretical and experimental imaging of a more asymmetric insulating surface, the CaF_2 (111) surface.

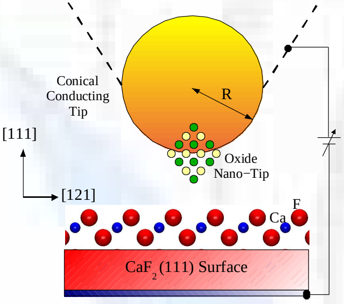
NC−AFM



- Tip−surface interaction causes a change in the frequency or **detuning** of oscillations.
- An image is generated by plotting the change from equilibrium frequency as the tip moves over the surface at a constant height.

Theoretical Setup

- Tip−surface interaction due to 3 components:
  - Microscopic forces between atoms in the tip and atoms in the surface − calculated by atomistic simulation.
  - Macroscopic van der Waals force between tip and surface − calculated analytically.
  - Electrostatic forces due to work functions, charging and polarization of conducting materials − calculated by a combination of atomistic simulation and analytical functions.



- Atomic nano−tip can be orientated to produce both a positive and negative electrostatic potential.

Disturbance in the Force

- Model the oscillations of the cantilever under the influence of total tip−surface force using experimental parameters.
- For stable imaging, experiments are setup so that any damping is cancelled by the external force. Also assuming F is independent of time we get:

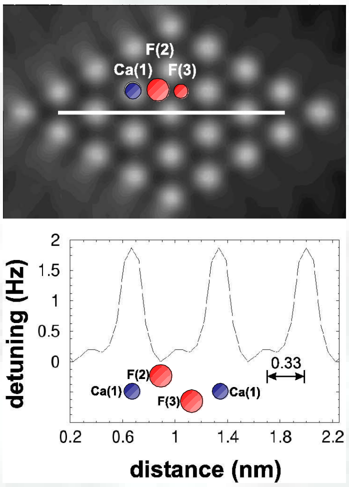
$$\ddot{z}+\omega_0^2 z-\frac{\omega_0^2}{k}F(z+h)=0$$

- Solve numerically to find the change in frequency for a given tip−surface separation.

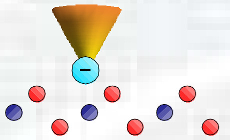
$$\Omega^2=1-\frac{1}{\pi k A_1}\int F(z+h)\cos(\tau)\,d\tau$$

- Calculate frequency change over whole surface unit cell → Simulated Image

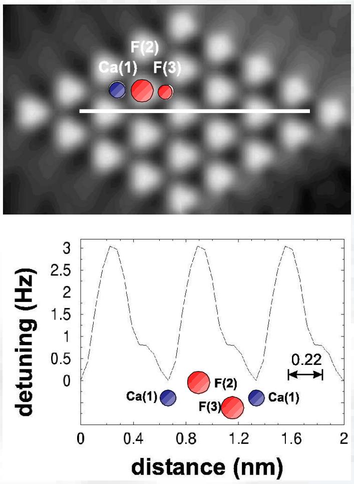
Theoretical Images



- Simulated image and scanline produced at a constant height of 0.4 nm over the CaF2 (111) surface with a nano−tip with a positive electrostatic potential. The white line is in the [121] direction and shows the position of the scanline.



Ca imaged as bright disks with negative potential tip.



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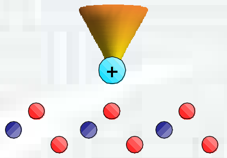


Both F ions imaged with positive potential tip, producing bright triangles.

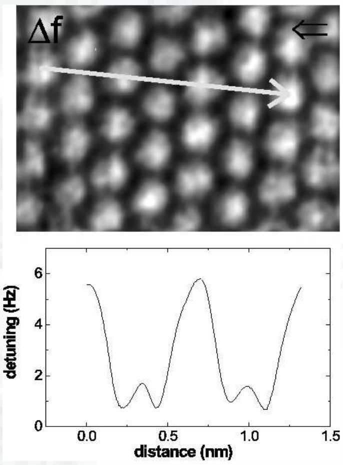
Statistics

- Statistical analysis of position of secondary peaks over many scanlines from 3 independent experiments shows very good agreement with simulation.

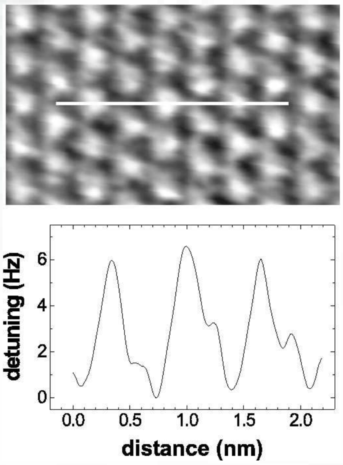
Contrast Pattern	Exp. 2nd peak position (nm)	Theo. 2nd peak position (nm)
Disk−like	0.32±0.05	0.33
Triangular	0.24±0.04	0.22

- The clear difference in 2nd peak position for the two different contrast patterns in both experiment and theory introduces quantitative evidence for interpretation.

Experimental Images



- Example experimental image and scanline taken at constant height. The white line is in the [121] direction and shows the position of the scanline. For this experiment the amplitude (A_1) was 24 nm and the equilibrium frequency (f_0) was 60 kHz.



- Example experimental image and scanline taken at constant height. The white line is in the [121] direction and shows the position of the scanline. For this experiment the amplitude (A_1) was 35 nm and the equilibrium frequency (f_0) was 77 kHz.

Summary

- By combining high quality experiment with theoretical simulation, for the first time, unambiguous interpretation of NC−AFM images of a binary insulator has been achieved.
- Simulation predicts two distinct contrast patterns dependent on the sign of the electrostatic potential from the tip:
  - A negative potential images the Ca^{2+} sublattice as bright and demonstrates a disk−like contrast pattern.
  - A positive potential images both F^- sublattices and demonstrates a triangular contrast pattern.
- Reproducible experimental images also demonstrate two distinct contrast patterns and a statistical comparison of features in simulated and experimental images show good agreement.

References

A. S. Foster, C. Barth, A. L. Shluger and M. Reichling − *Phys. Rev. Lett.* **86** (2001) 2373
C. Barth, A. S. Foster, M. Reichling and A. L. Shluger − *J. Phys.: Condens. Matter* **13** (2001) 2061