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# Tenkých vrstev a nanostruktur

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TÉMA

## Simulating atomic force microscopy of calcite in water

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The atomic force microscope (AFM) can be operated in liquid environments, where it can be used to image flat surfaces with high resolution, study the structure of hydration layers, or image and manipulate biological systems on the nanoscale [1]. However, in all these situations, the tip-surface interaction mechanism is more complicated than in vacuum or air, and therefore generally not well understood.

We chose the calcite (10-14) surface as a model system for our simulations. Although recent atomically resolved non-contact AFM images of calcite in water [2] resemble those obtained in UHV [3], the imaging mechanism in liquid is more complicated [4], due to the presence of hydration layers around the tip and above the surface, which leads to significant entropic contributions to the force on the AFM tip.

The system, consisting of several layers of surface material, water, and the tip apex represented by a nanocluster, is described by empirical atomistic interaction potentials [5]. We use (N,V,T) - molecular dynamics and umbrella sampling to compute continuous free energy profiles of the system, as a function of the tip-surface separation, for different lateral tip positions. The derivative of the free energy with respect to the tip-surface distance is the best estimate for the force acting on the AFM tip, as the entropic contributions from interactions of hydration layer water molecules are correctly taken into account.

Finally, we use the virtual AFM, recently developed in our group, to simulate the full AFM cantilever oscillation in the force field obtained from the free energy calculations, matching the experimental parameters for oscillation frequency and amplitude, as well as the cantilever's stiffness and quality factor. The images obtained from these simulations agree very well experiment, validating our approach.

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