Role of the tip in NC-AFM energy dissipation

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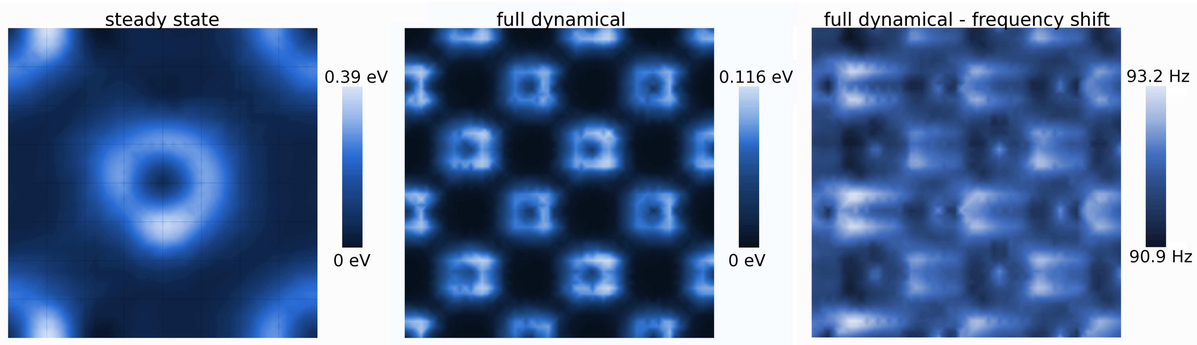
Introduction

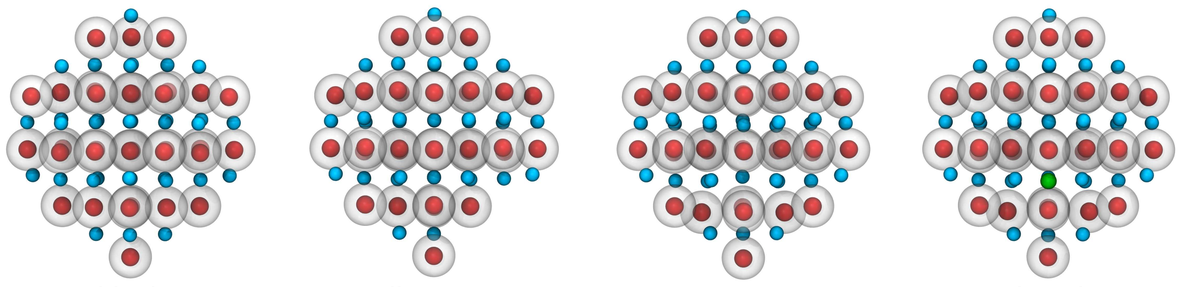
- NC-AFM frequency shift and topography measurements are well understood.
- Damping signal has sometimes better resolution.
- It can even show different patterns in the image.
- Unfortunately it is not that well understood!
- We use different methods to theoretically study the dissipative processes and aid experiments interpretation.

Images



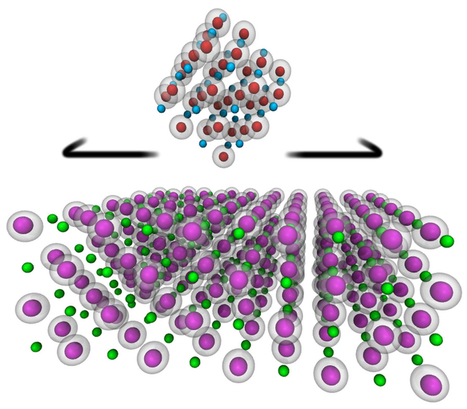
- The order of magnitude and the surface pattern of dissipation signal is in good agreement with typical experiments.
- At finite scan speed, the frequency shift image looses spatial resolution and the contrast appears inverted; the dissipation signal does not change dramatically: better resolution.
- The ring shape in the dissipation images is an artefact of the atomistic potentials.

Static Approach

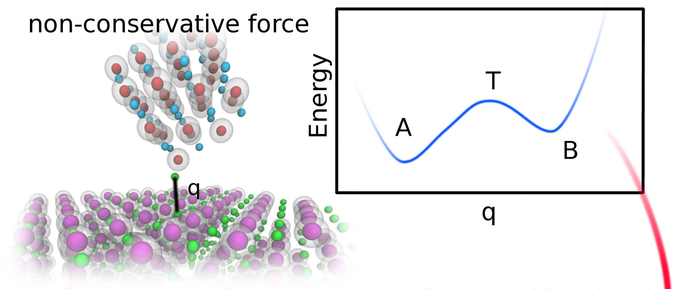


We tested these tip geometries with different materials: MgO, NaCl and KBr

conservative force



non-conservative force



With atomistic calculations we get the forces acting on the tip in several positions and build a 3D forcefield.

At close approach we compute the transition barriers of the most unstable surface atom. We build a 3D dissipative field describing the transition rates.

$$W_{AB}(z) = \nu_A(z)\exp[-\beta\Delta E_{TA}(z)]$$

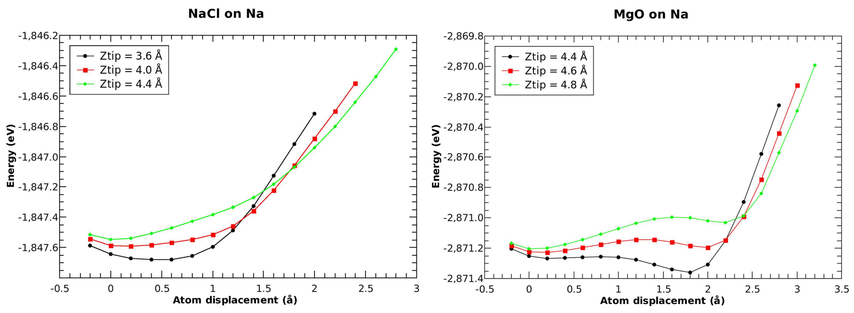
The rates will be used to integrate the probability of being in either A or B.

$$\frac{dP_A(t)}{dt} = -P_A(t)W_{AB} + P_B(t)W_{BA}$$

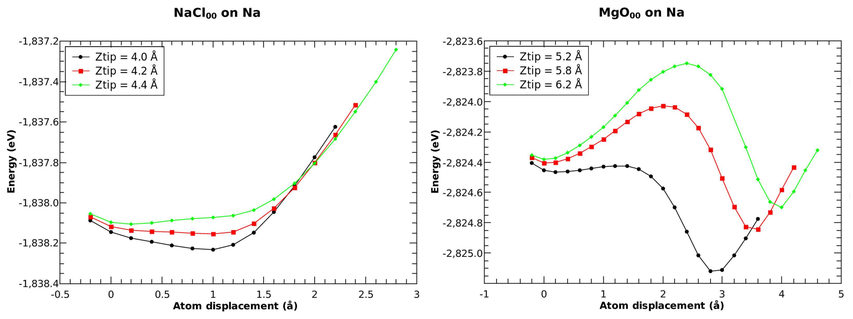
Finally the force acting on the tip is given by:

$$F_m(z,t) = P_A(t)F_A(z) + [1 - P_A(t)]F_B(z)$$

Our virtual machine uses the conservative forcefield and the dissipative field to simulate the cantilever motion in a dynamical AFM experiment.



Ideal NaCl tip does not produce the state B.

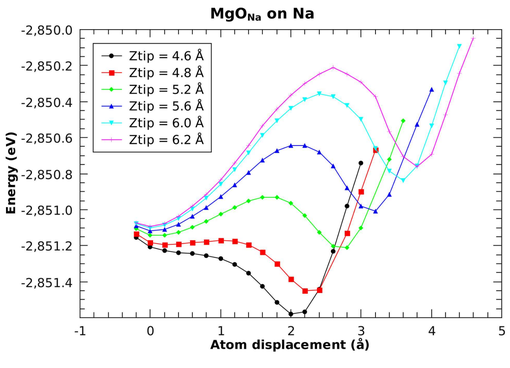


Ideal MgO tip has both states in a very small range of tip heights.

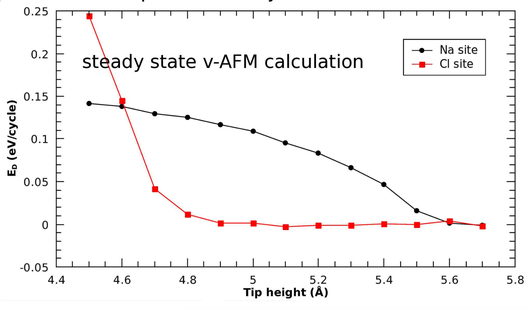
Divacant NaCl gives the state B but in a small region of tip heights.

Divacant MgO has both A & B but now B is the groundstate, i.e. the surface atom will get stuck on the tip.

Vacant tips behave like these.



The doped MgO tip gives both minima A & B in a sufficient portion of the tip oscillation cycle.

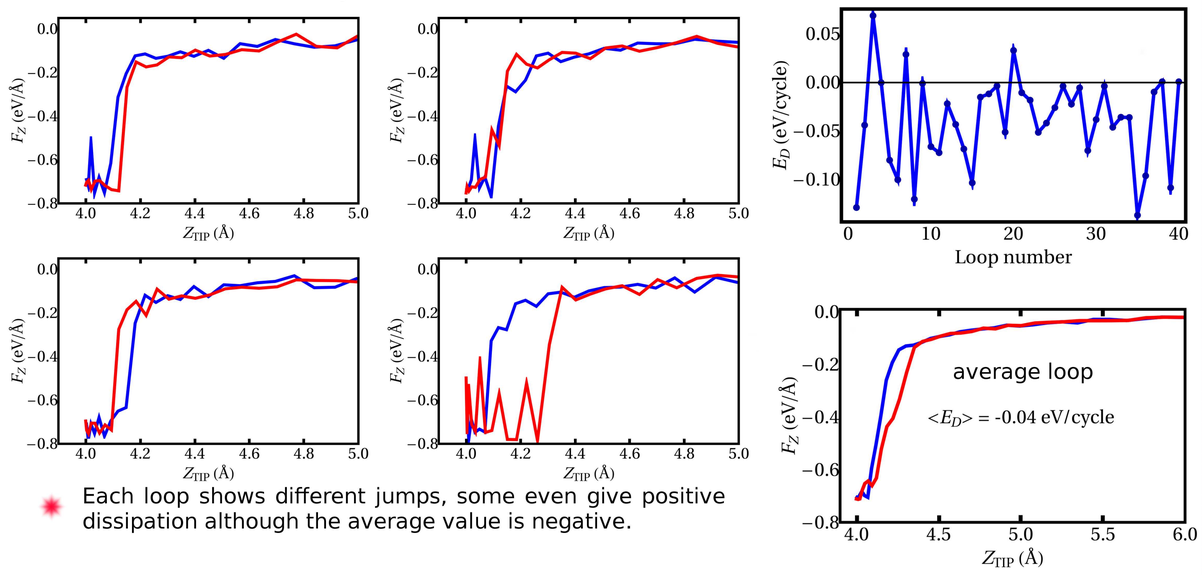


Beyond the Static Approximation

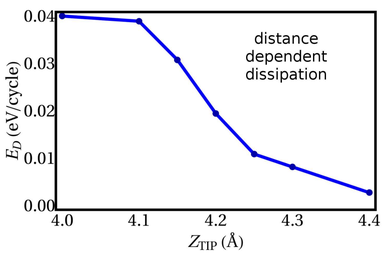
- Theory of Dynamic Response models the dissipative process as statistical jumps of a single degree of freedom, calculated at 0 temperature.
- A Molecular Dynamics simulation includes all the degrees of freedom, but it will be more computationally demanding.

The CUstic MD program running on Tesla GPU can be x100 faster than a conventional atomistic code

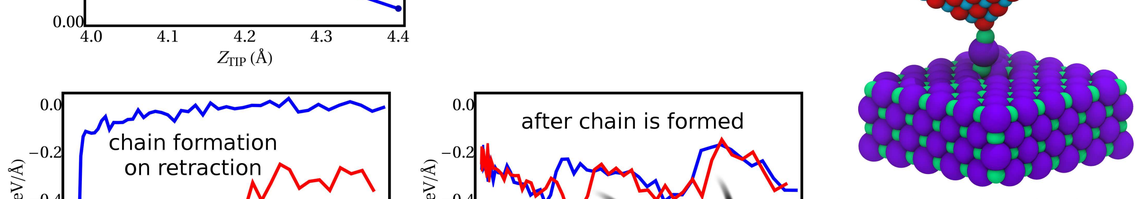
Accelerating oscillation frequency (150 MHz), computing only lower part of the loop reduces simulation time to ~0.5 ns/cycle = ~20 mins wall time.



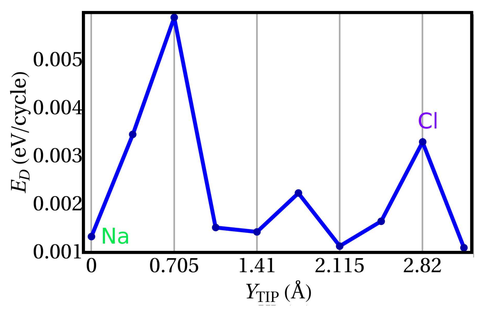
Each loop shows different jumps, some even give positive dissipation although the average value is negative.



The MgO tip makes the surface atoms unstable and it is possible to see the statistical jumps of the closest Na atom, mainly responsible for the dissipation.



but when the tip is a bit displaced from Na sometimes we see tip changes and chain formation. Dissipation is seen also after the chain is formed.



In MD simulations the ideal NaCl tip gives a very small dissipation (~3 meV/cycle) after averaging more than 60 loops. The tip is stable in every position.

The NaCl tip gives minimal perturbation and the dissipation comes from the weaker jumps of all the atom close to the tip.

Tips that were predicted to be too stable in the static calculations, give a considerable dissipation in MD, while the ones predicted "optimal" are now too reactive.

This approach ensures a better probing of the statistics but is more expensive.