ATOMIC SCALE ENERGY DISSIPATION MECHANISMS IN NON-CONTACT ATOMIC FORCE MICROSCOPY

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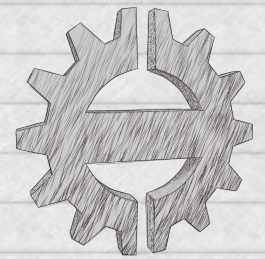
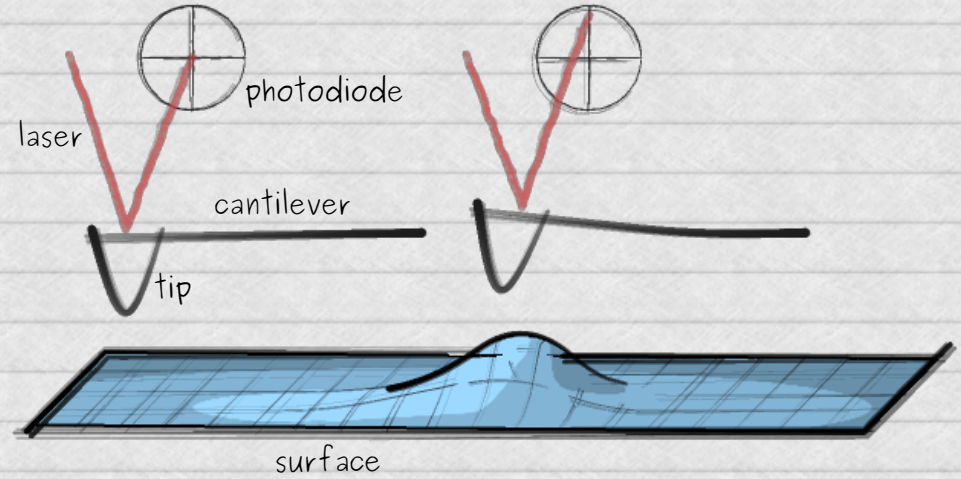


INTRODUCTION

The Atomic Force Microscope (AFM) measures the interaction between a tip and the sample through the deflection of a cantilever.



Constant height or constant deflection (topography) modes...

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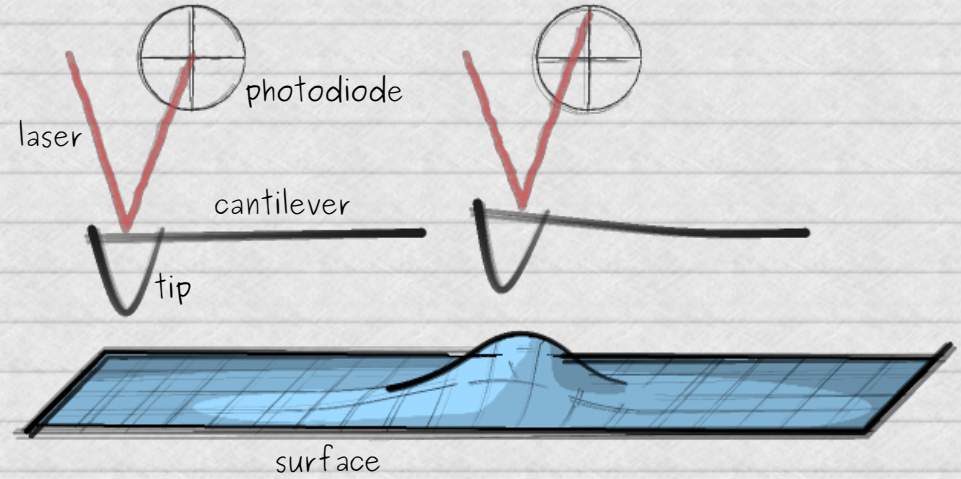
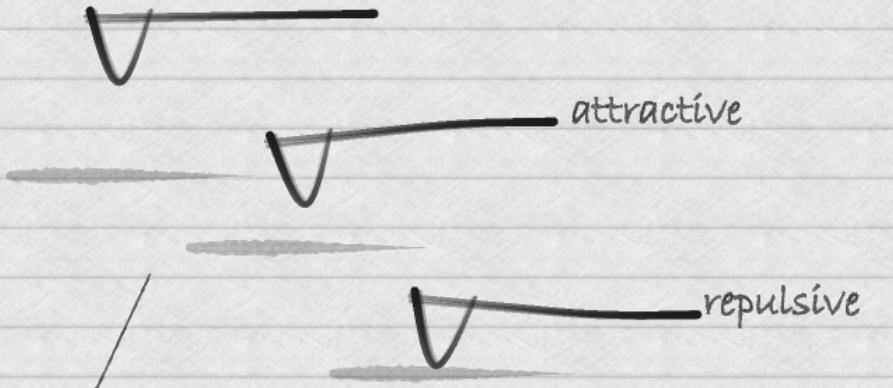
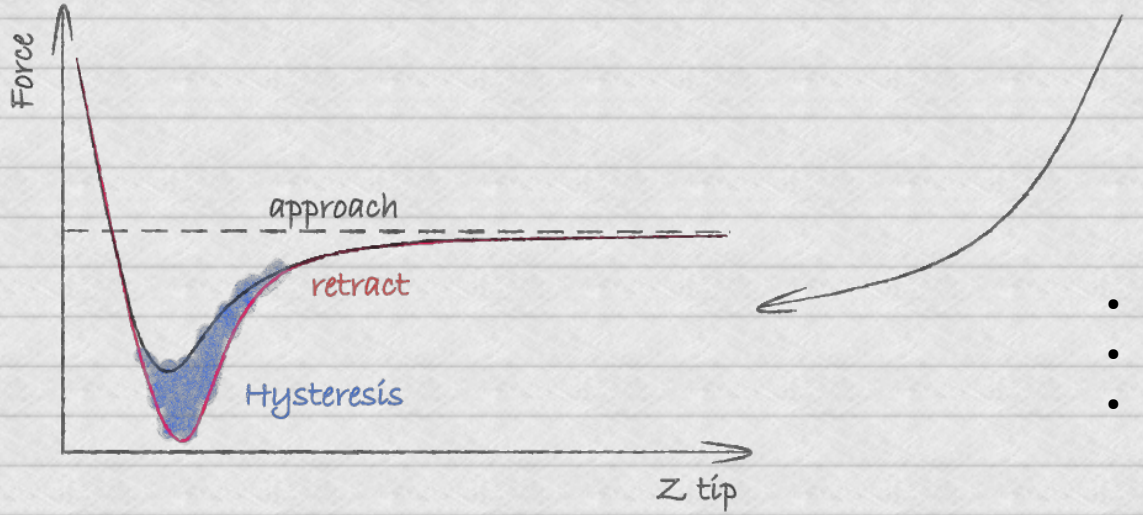


Constant height or constant deflection (topography) modes...



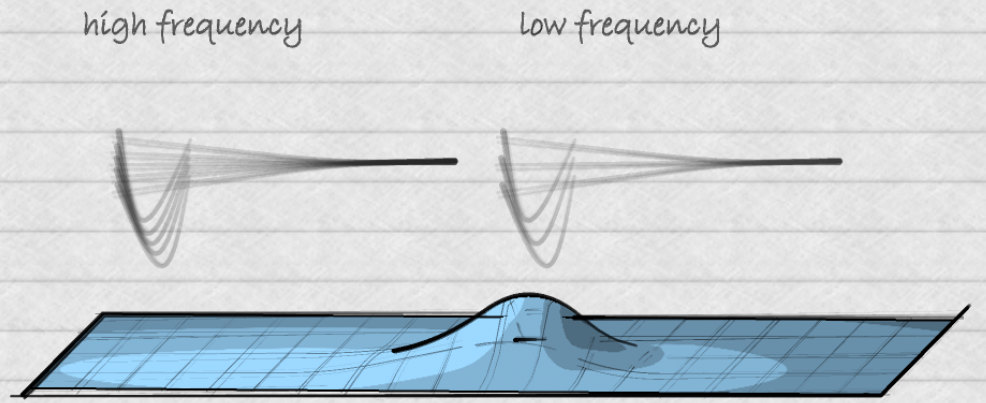
... or we can measure Force VS. Distance



- see adhesive processes
- low resolution!
- tip/surface damage!

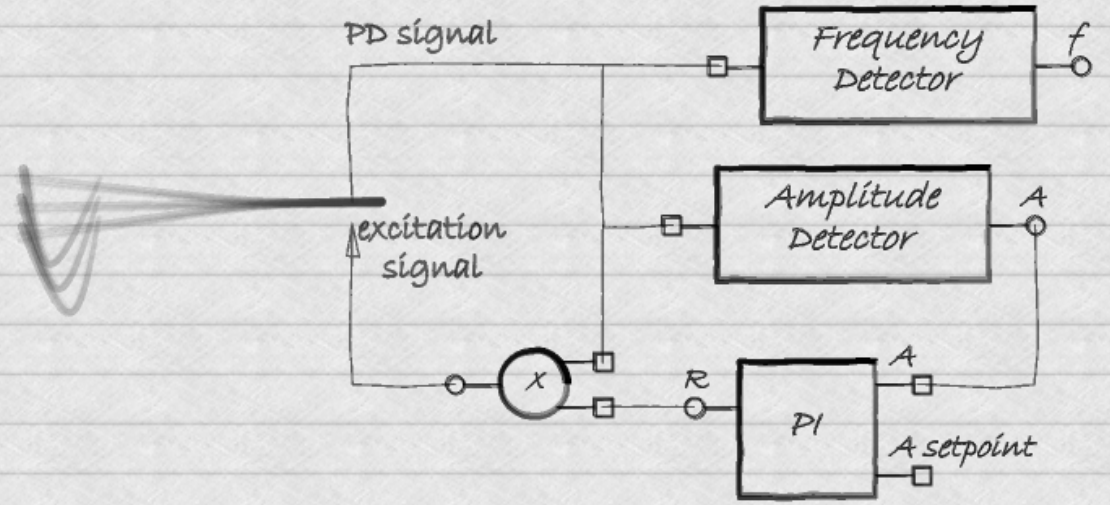
INTRODUCTION

Non-Contact Atomic Force Microscopy also provides topography and 3D force maps with atomic resolution.



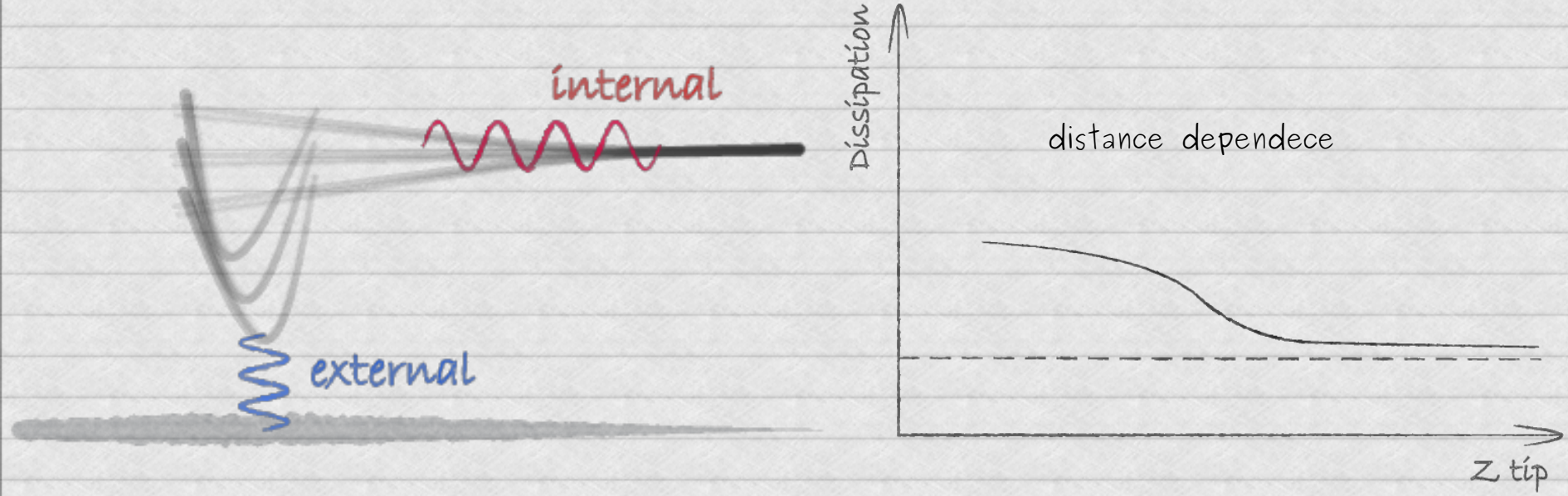
- oscillating cantilever
- constant amplitude (usually)
- $\Delta f \leftrightarrow$ force
- self-excited

- complex setup
- heavy averaging
- little tip/surface damage
- true atomic resolution!



INTRODUCTION

The excitation **R** is a measurement of the mechanical energy **ΔE** lost by the system during the oscillation cycles.



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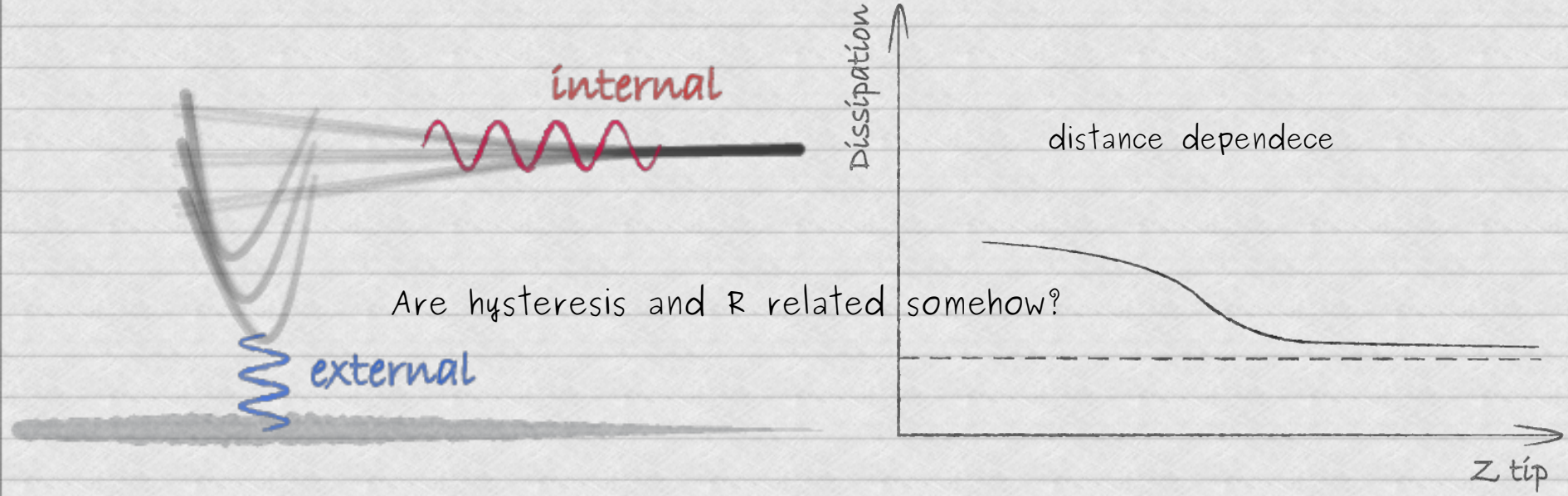

Are hysteresis and R related somehow?

... and why bother?

INTRODUCTION

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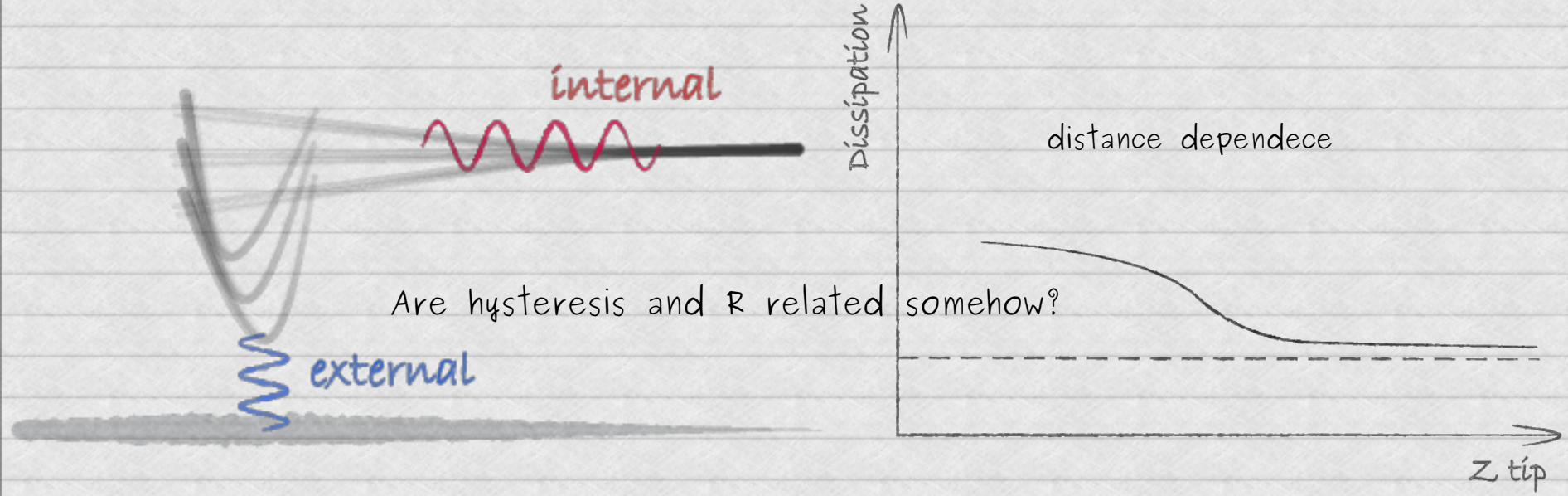
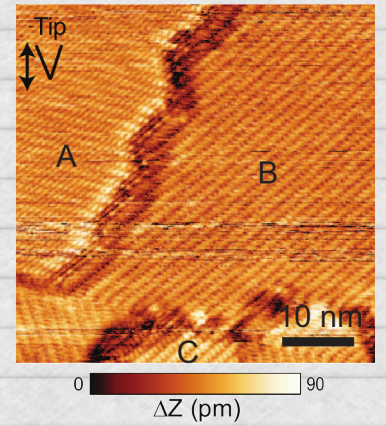
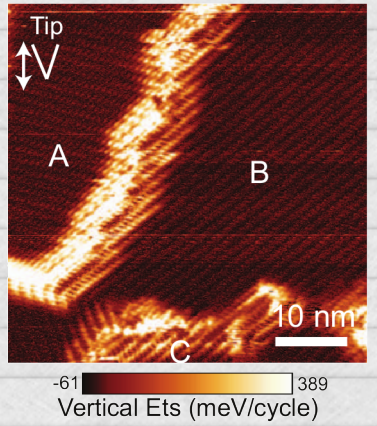


topography



dissipation



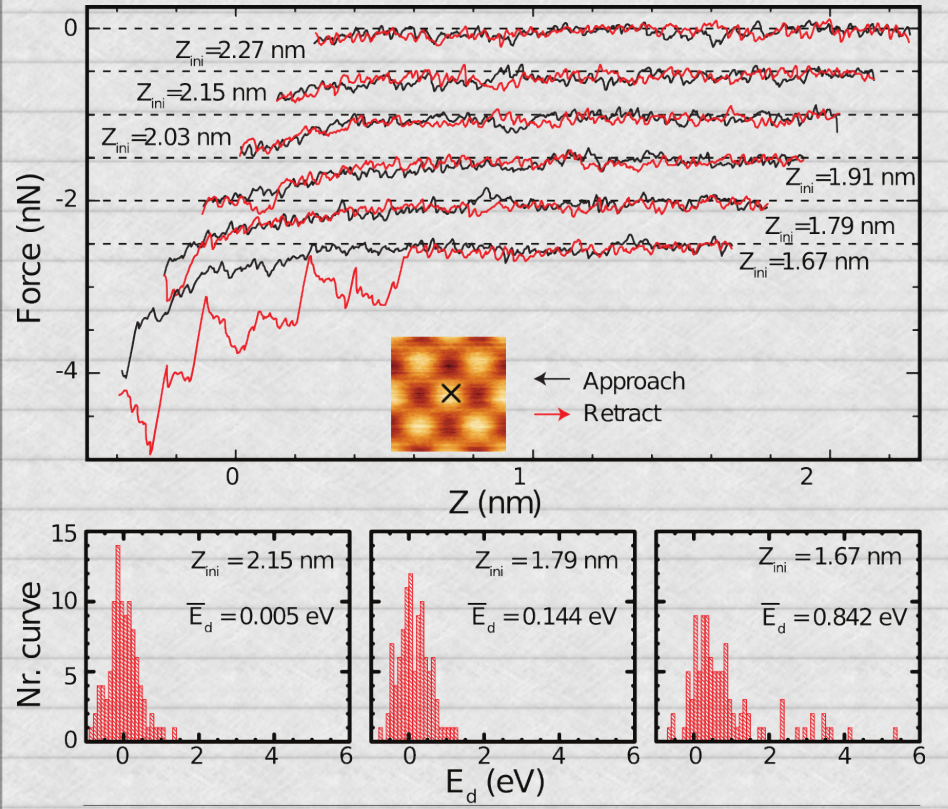
... and why bother?

- often Δf ≠ ΔE
- sometimes Δf = 0
- Dissipation is not well understood!
- access to new physics?

EXPERIMENT

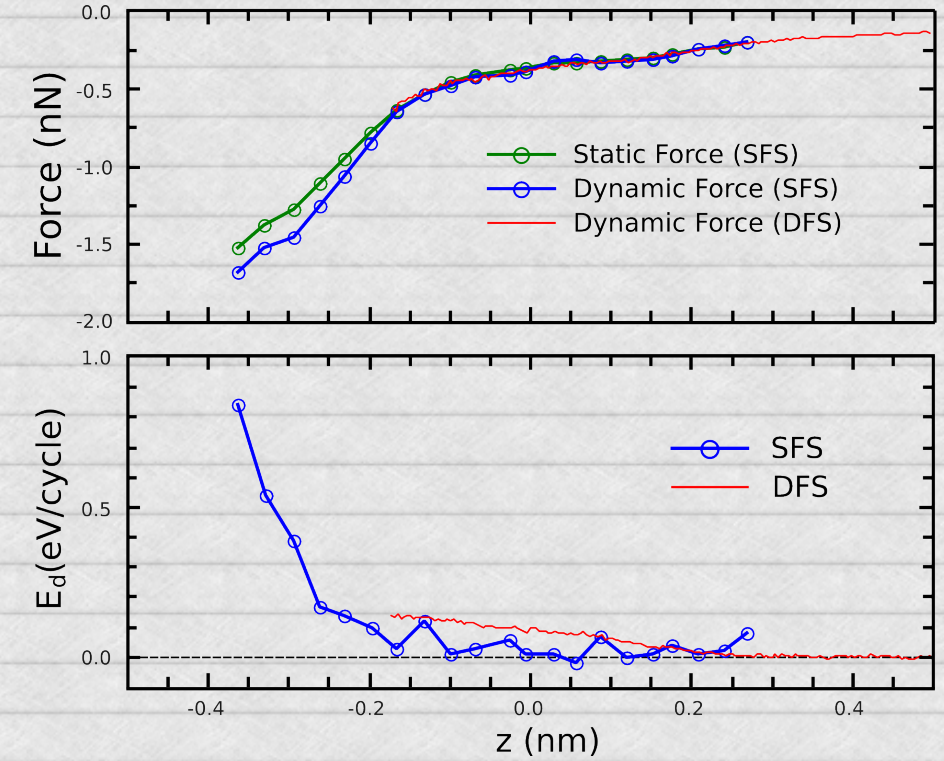
The studied system is an NaCl (001) flat surface. The Si tip was crashed in the surface before measuring.

Static Force Spectroscopy



- No surface damage / tip change
- Stochastic behaviour
- Average hysteresis → dissipation

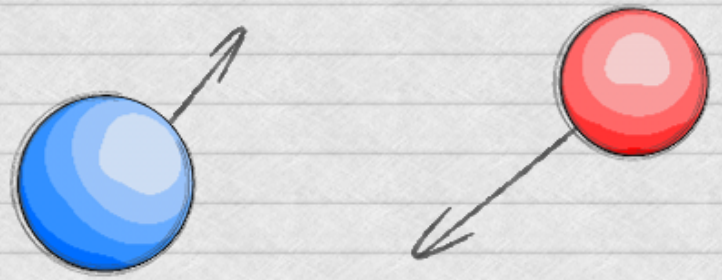
Dynamic Force Spectroscopy



- DFS & SFS force agree well
- Dissipation not so much!

SIMULATION

The idea is to simulate one oscillation cycle, get the force curve and its hysteresis.



$x \rightarrow x + vt + at^2/2$

Full dynamical simulation is required:

- molecular dynamics
- tip oscillation

... a new code is needed!

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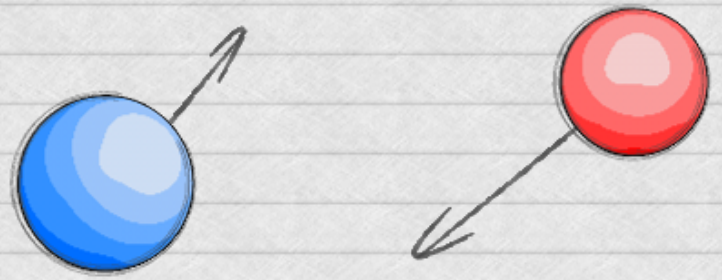

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Full dynamical simulation is required:

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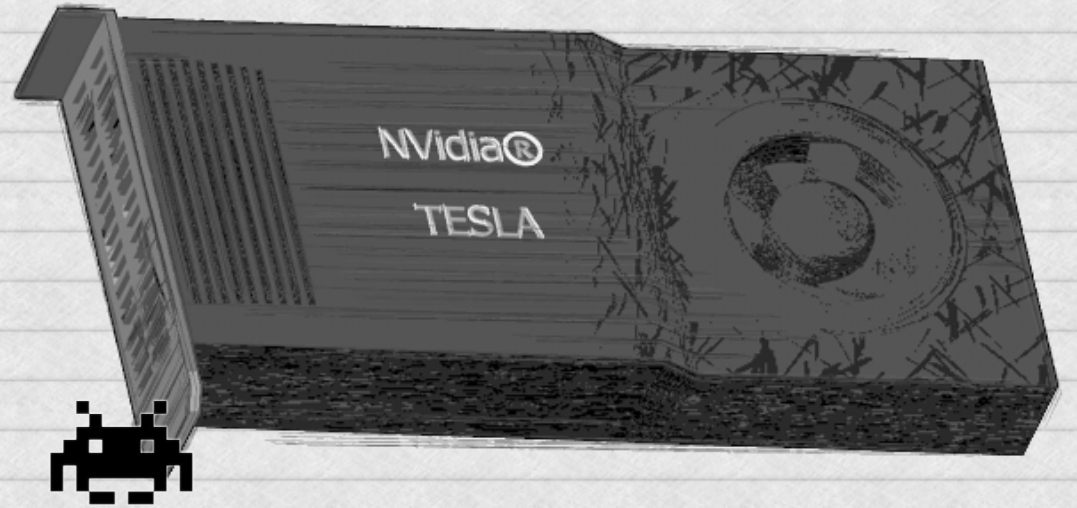
Full GPU implementation is +100x faster!

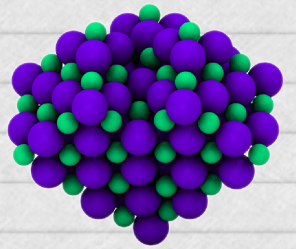
- max 12000 threads
- one thread per atom
- => 20 systems in one run!

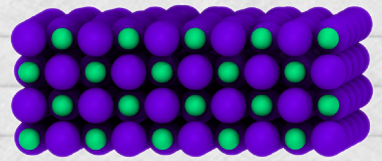


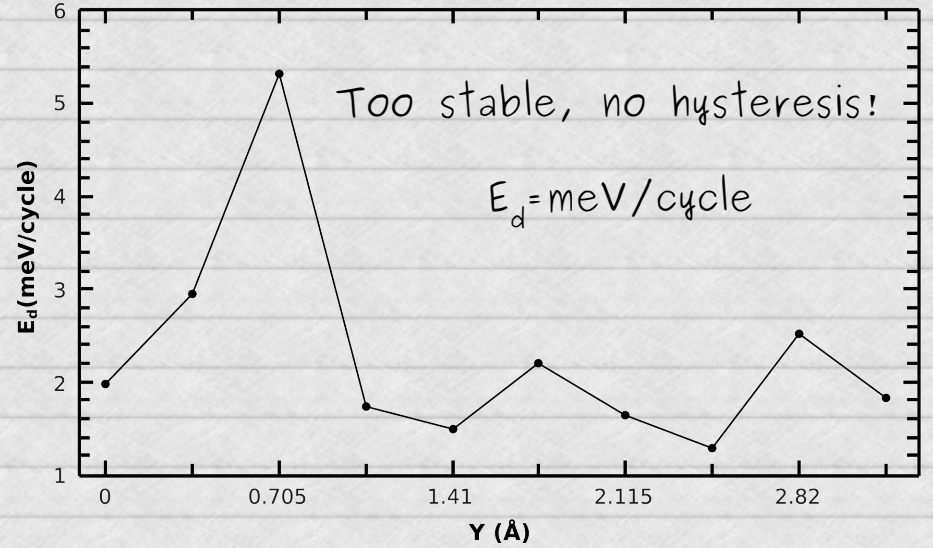
SIMULATION

Then we build a model for the tip and the surface. (Preferably NaCl based)

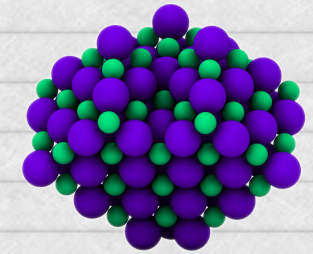
Basic tip: 4x4x4 NaCl cube
+ thermostat + holder







Basic tip, apex cut



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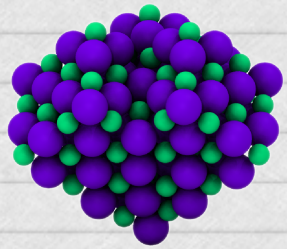

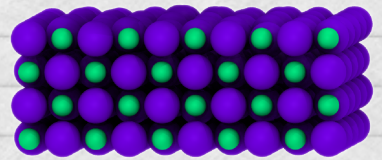

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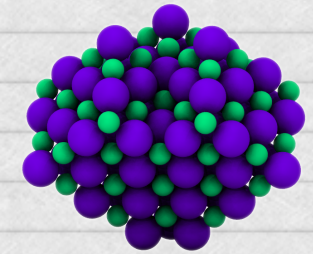

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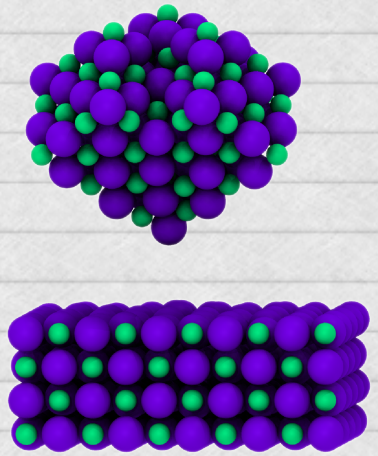

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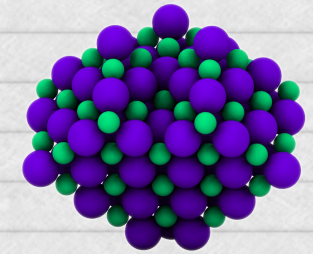

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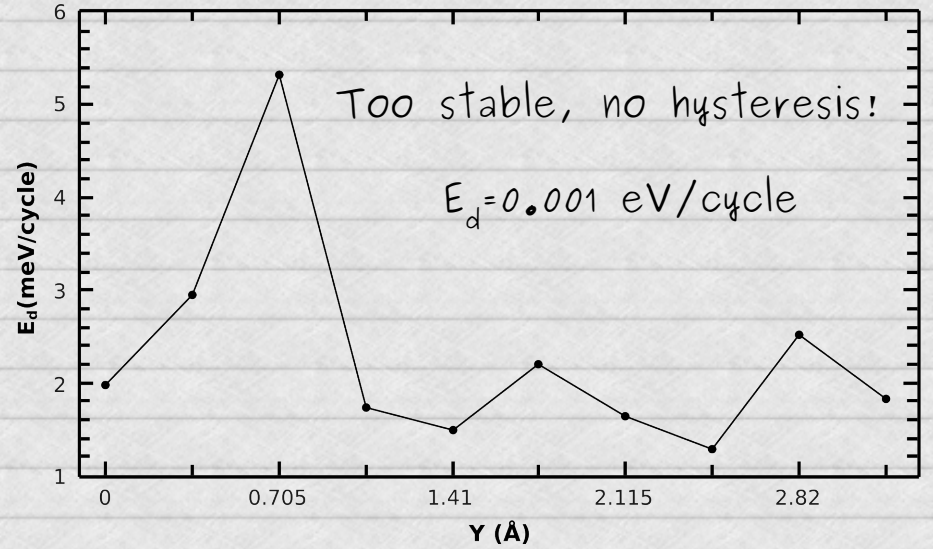
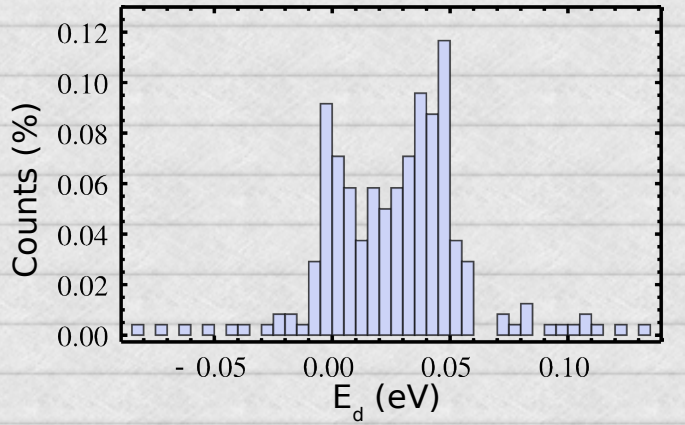


- Main process: atom adsorption is reversible
- Other process: displacement of second layer
- <E> = 0.02 eV/cycle still too small
- Max E for all the cycles is 0.08 eV



SIMULATION

Let's try an MgO tip instead.

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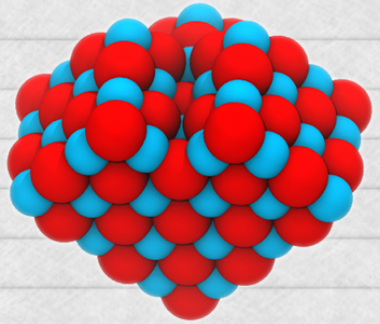

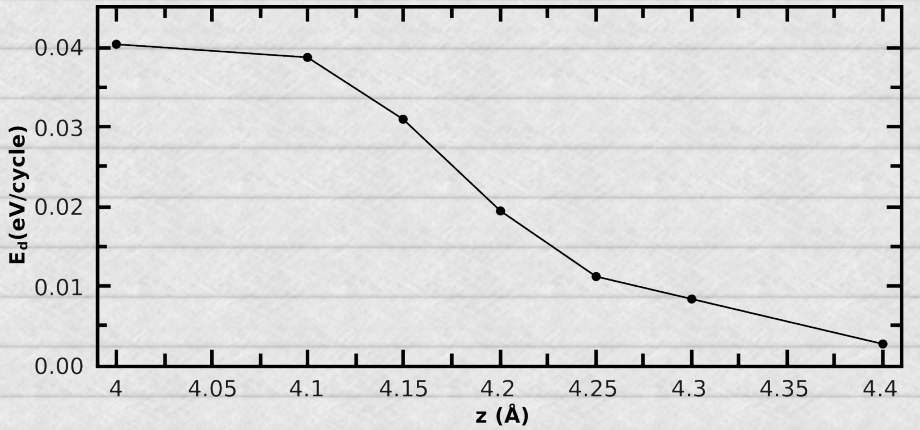

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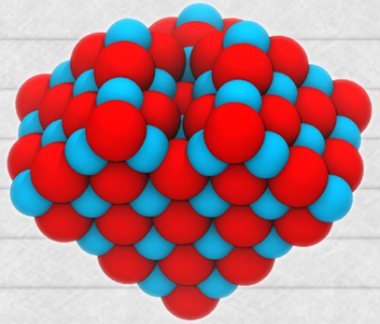
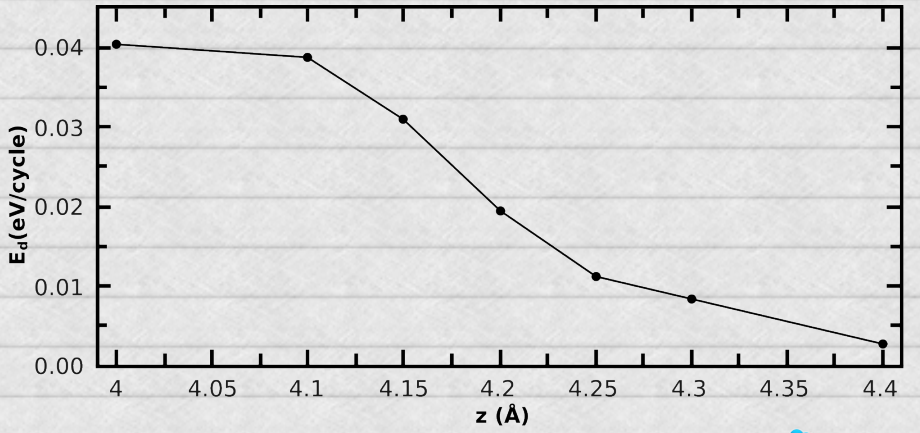
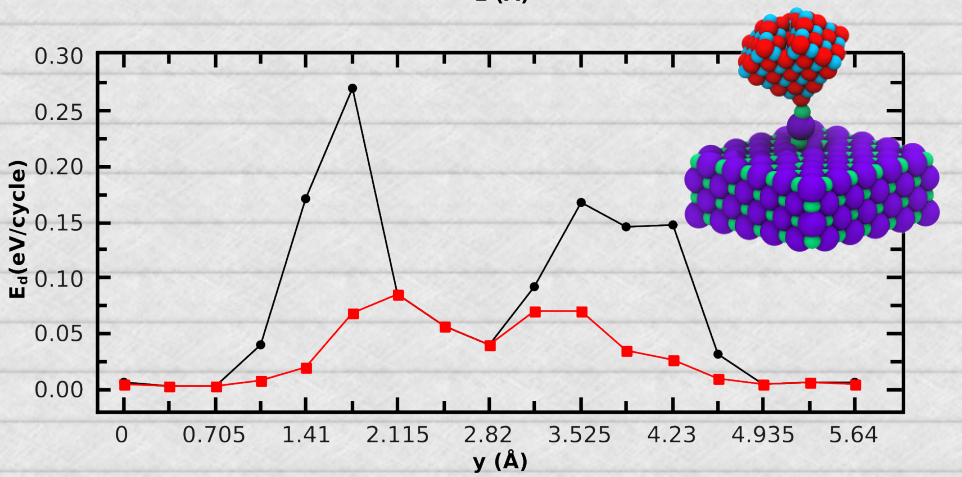
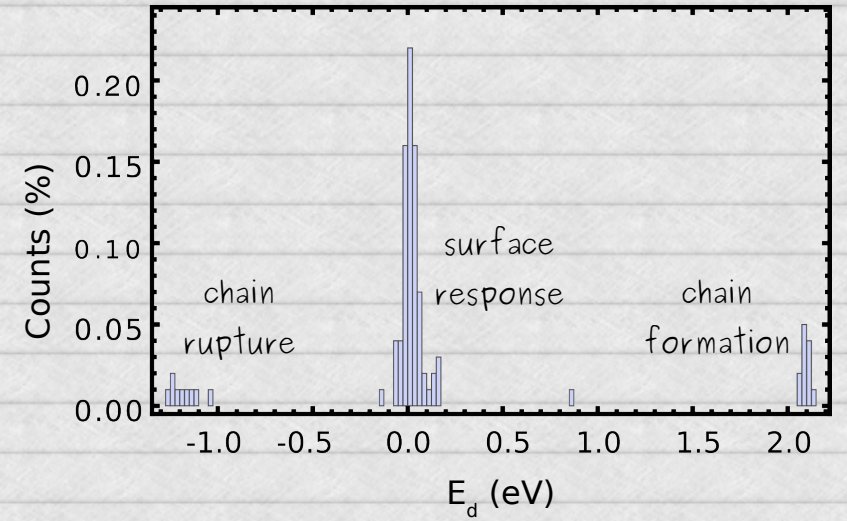






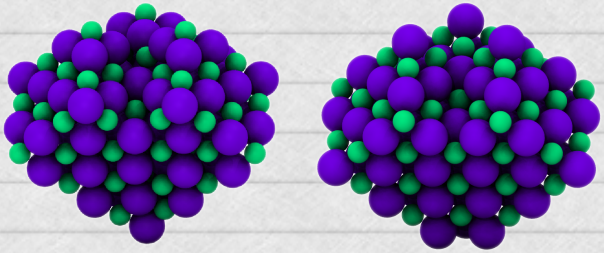


- nice z dependence on the active site
- the tip pulls chains from the surface
- probable surface decoration

SIMULATION

These tips failed!

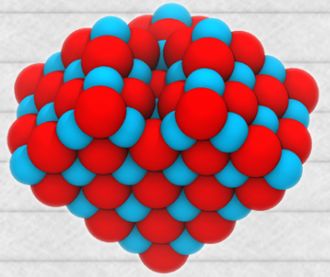
Simple NaCl based tips



...

Too stable / different mechanisms

Simple MgO tips

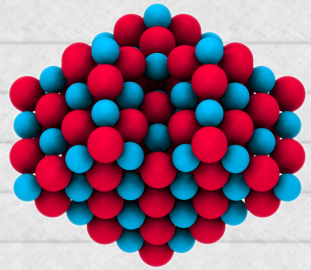


Too unstable / different mechanisms

We need a more realistic tip.

SIMULATION

Let's make the tip the "real" way!



Basic MgO...

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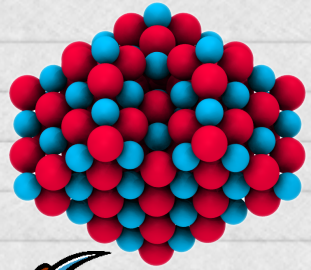
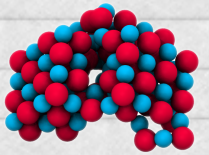
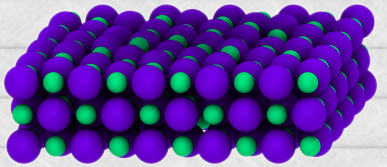


Basic MgO...

roughening...





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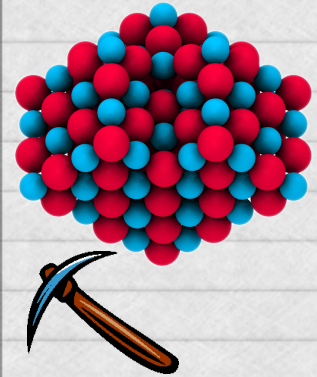

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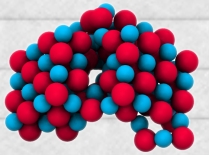
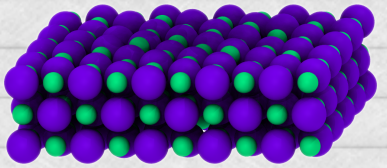
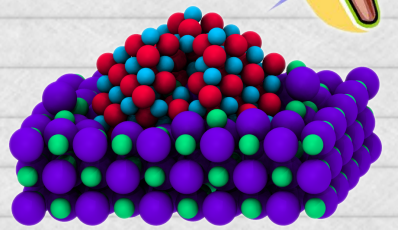




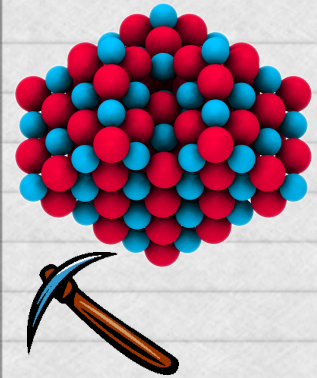
indentation...



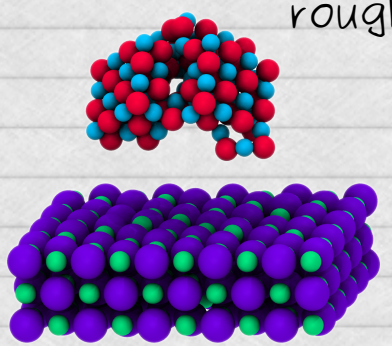
Slow AFM cycle close to the surface.

SIMULATION

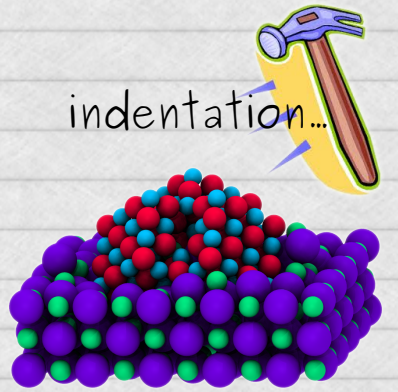
Let's make the tip the "real" way!



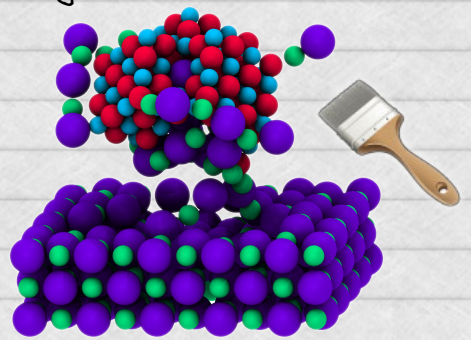
Basic MgO...



roughening...



indentation...

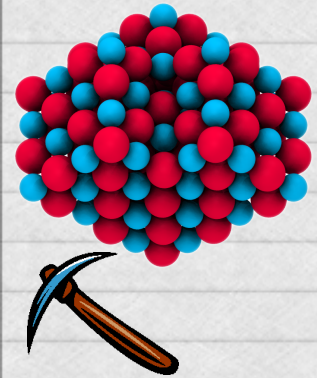


cleaning...

slow AFM cycle close to the surface.

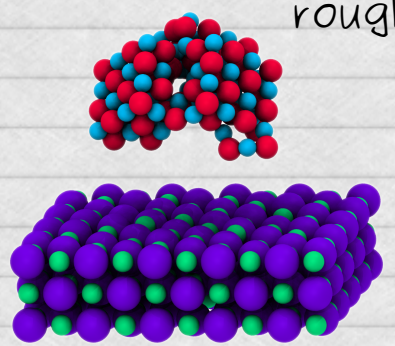
SIMULATION

Let's make the tip the "real" way!



Basic MgO...

roughening...



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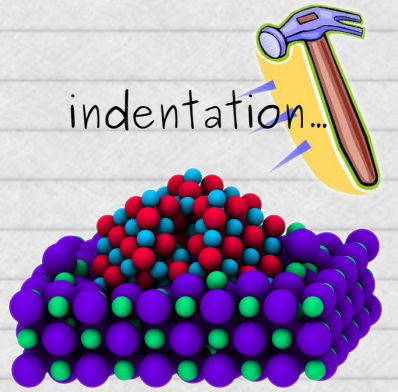

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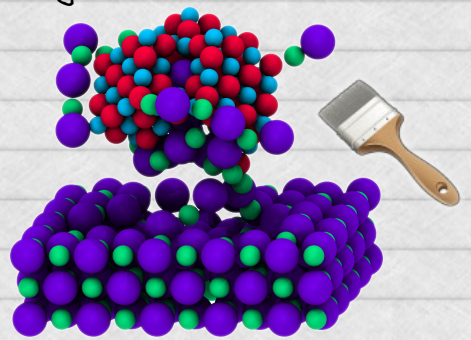


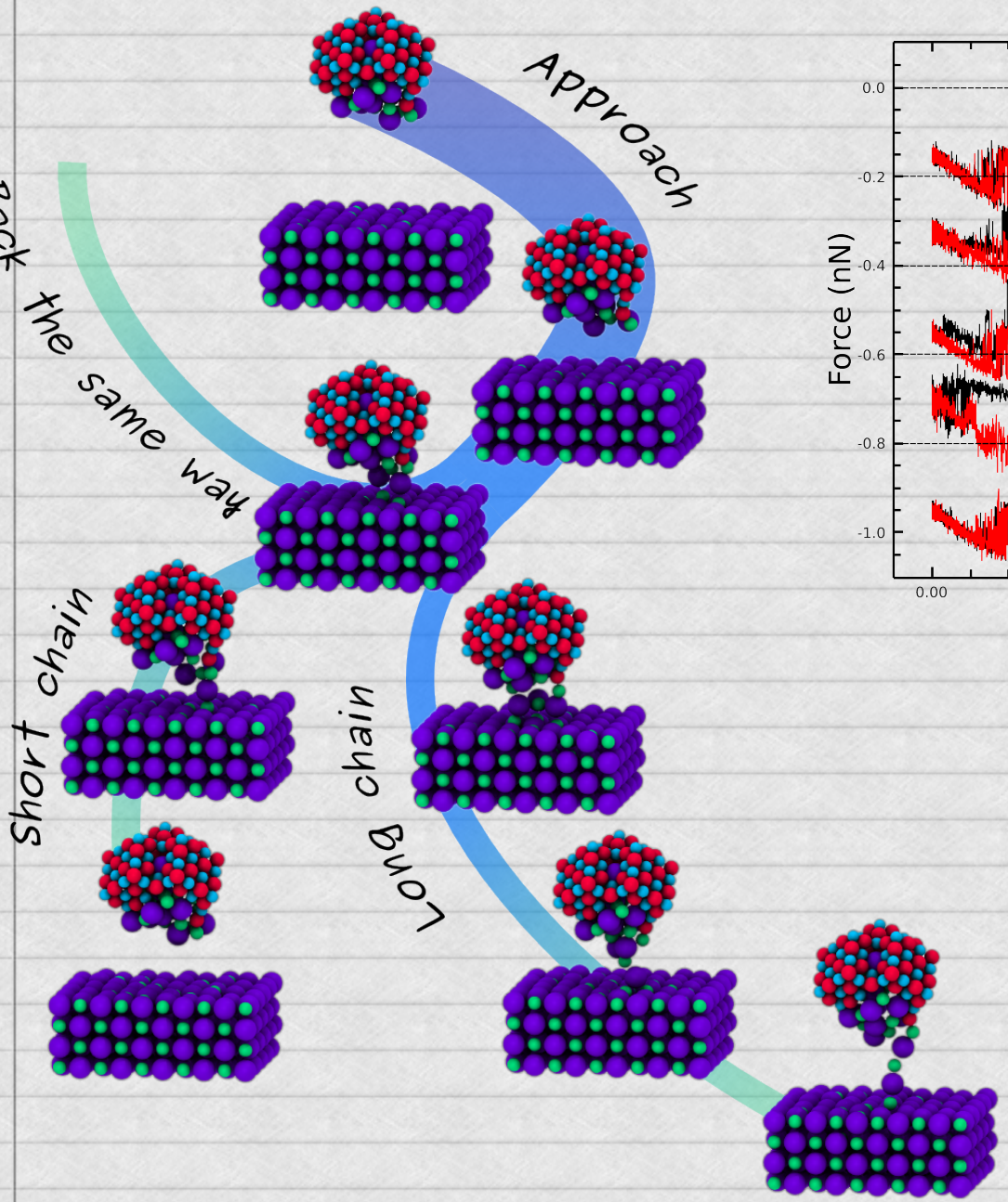
Oxide+NaCl nanocluster

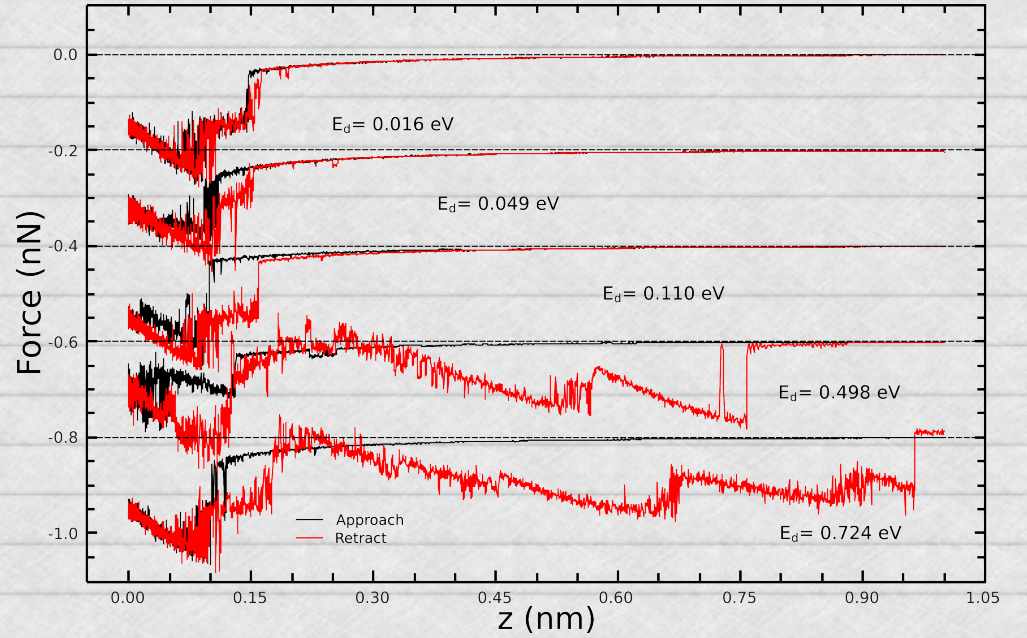
+ 1 ns relaxation

Slow AFM cycle close to the surface.

SIMULATION

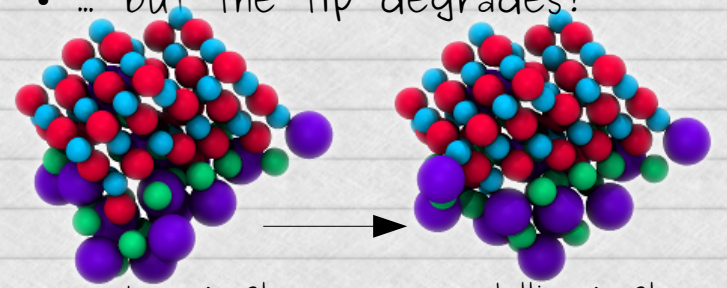
With this tip we simulate many cycles with different approach distances.





- stochastic behaviour
- tip chain formation
- No surface damage

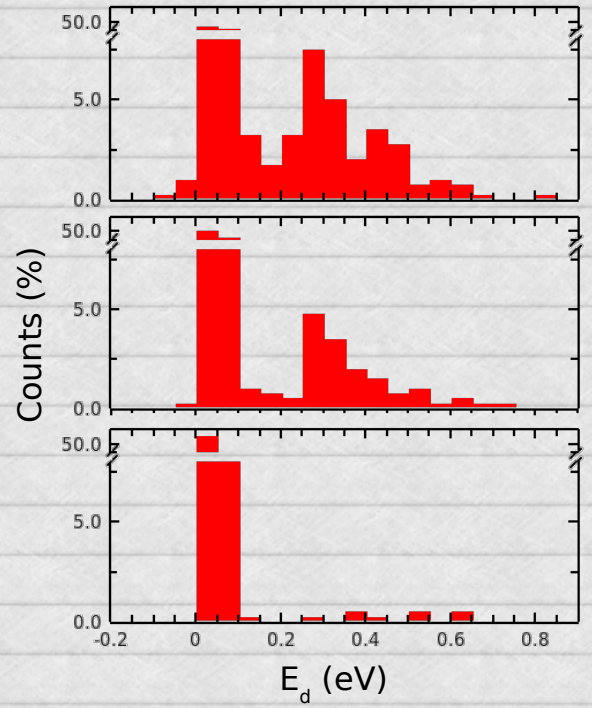
- … but the tip degrades!



amorphous NaCl
=> chains

crystalline NaCl
=> no dissipation

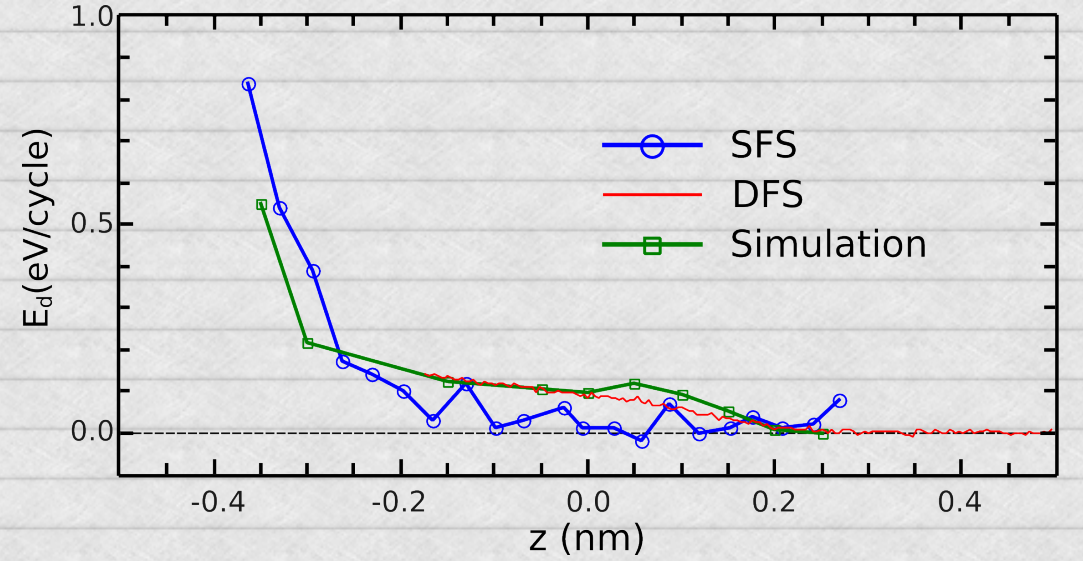
SIMULATION



5.5Å — Many chains at close approach

6.0Å — Infrequent chain formation increases the overall dissipation.

6.5Å — Very few chains far away



100 samples/point

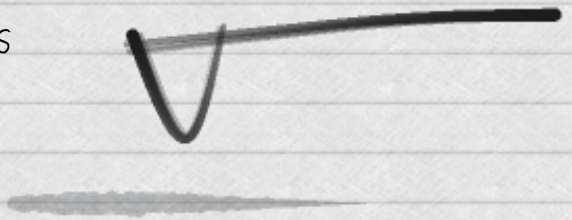
>1000 samples/point

400 samples/point

Simulated dissipation agrees with DFS!

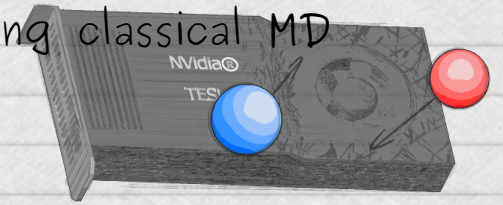
CONCLUSION

- SFS provides great insight in the dissipative processes

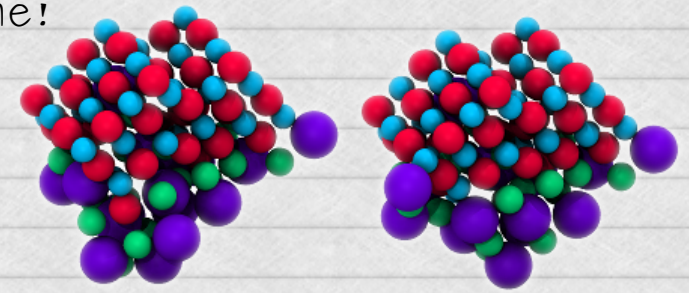


- DFS automatically averages whatever process is happening

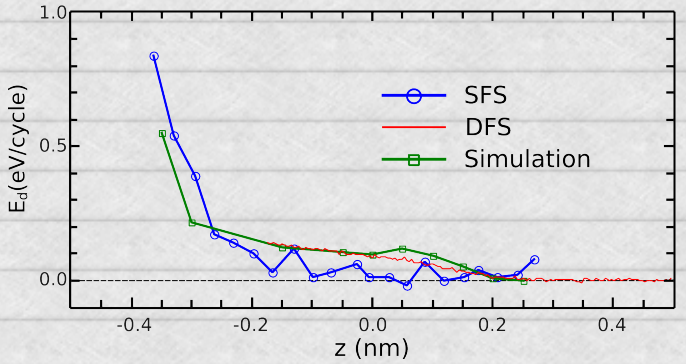
- We were able to simulate the same dissipative process using classical MD starting from the tip formation



- Our tip is smaller than the real one: degrades in time!



- Good quantitative agreement too!



CONCLUSION

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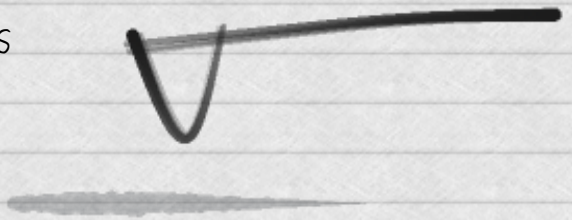

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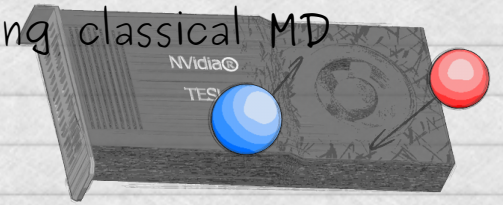

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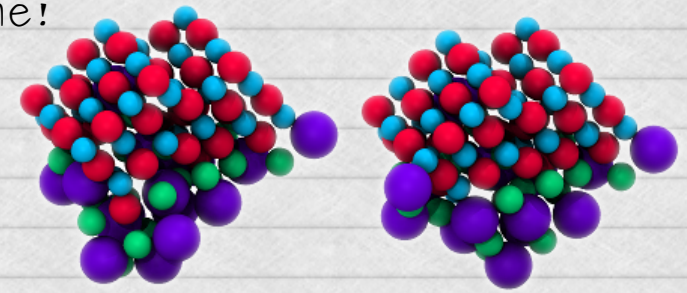

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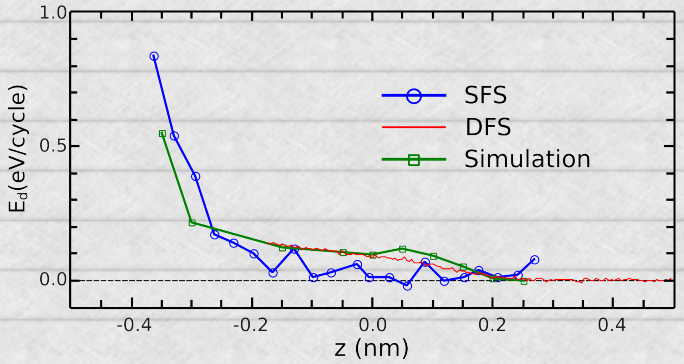

THANK YOU!