Determination of tip structures in atomic force microscopy

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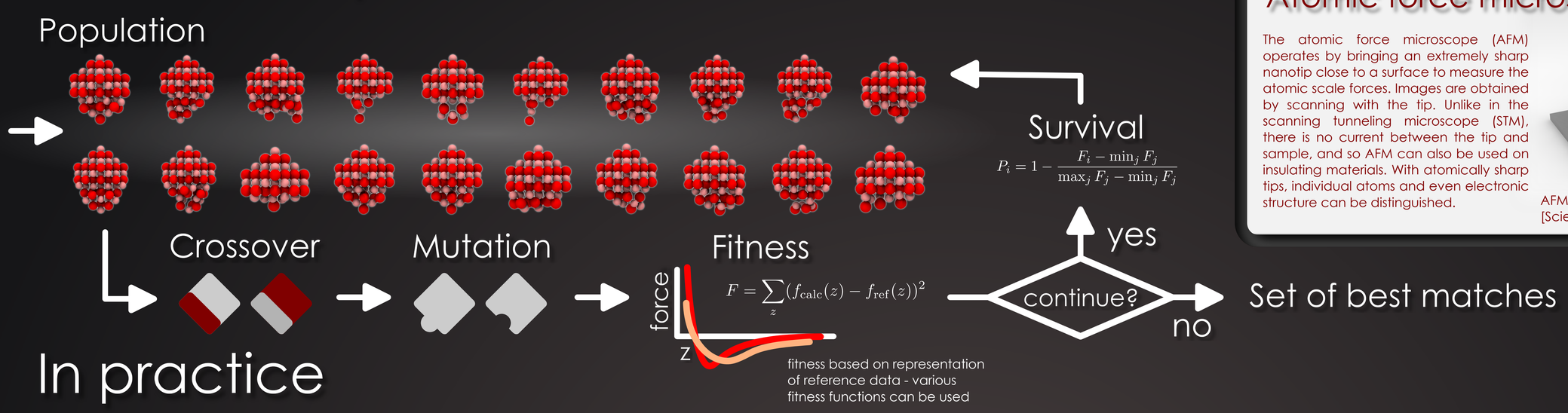
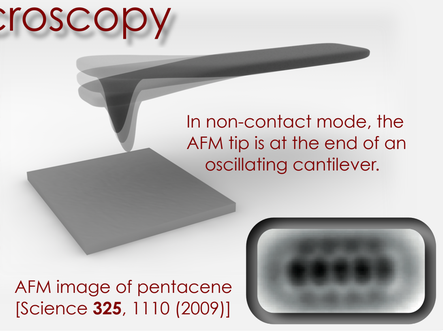
Evolutional optimization



fitness based on representation of reference data - various fitness functions can be used

Atomic force microscopy

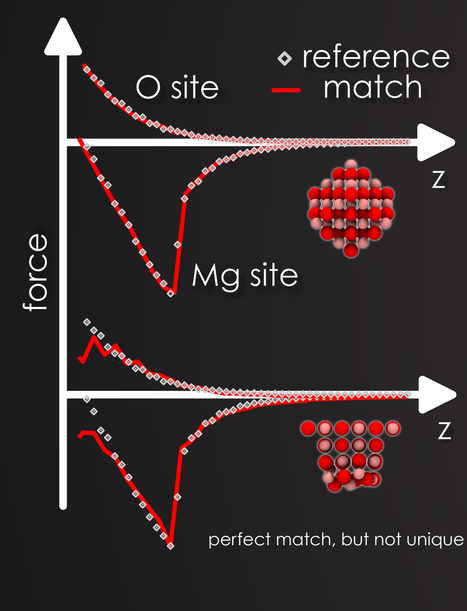
The atomic force microscope (AFM) operates by bringing an extremely sharp nanotip close to a surface to measure the atomic scale forces. Images are obtained by scanning with the tip. Unlike in the scanning tunneling microscope (STM), there is no current between the tip and sample, and so AFM can also be used on insulating materials. With atomically sharp tips, individual atoms and even electronic structure can be distinguished.



AFM image of pentacene [Science **325**, 1110 (2009)]

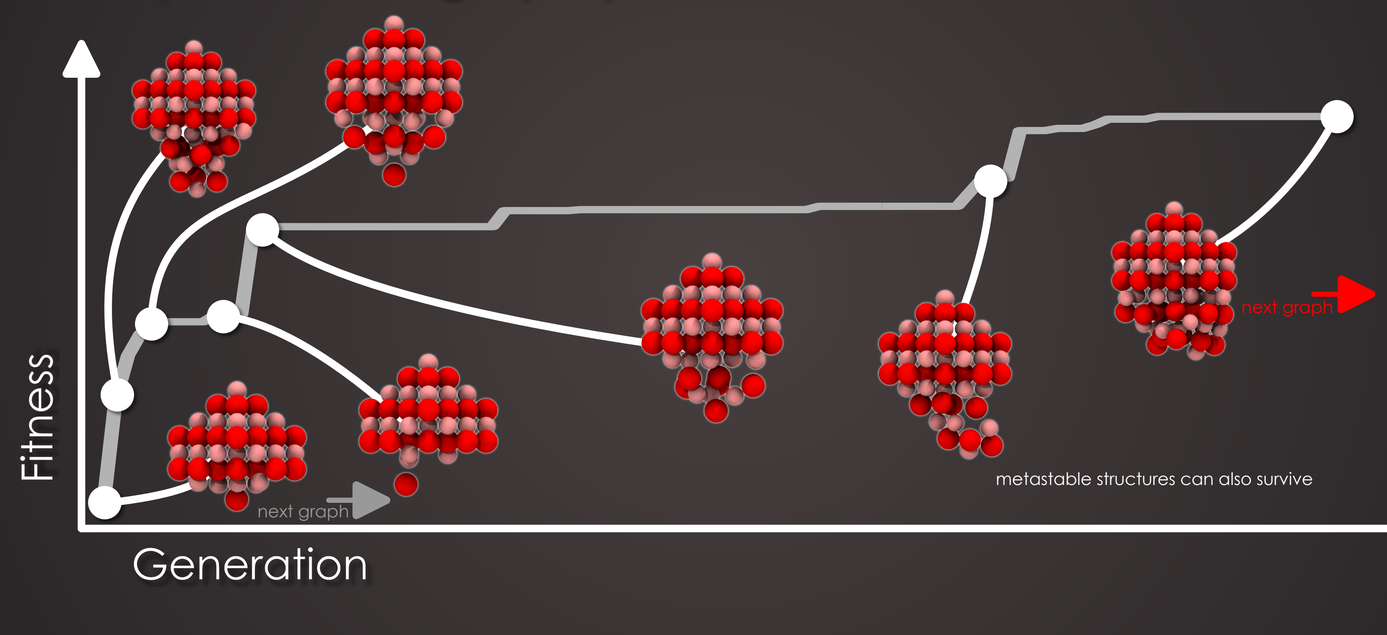
In practice

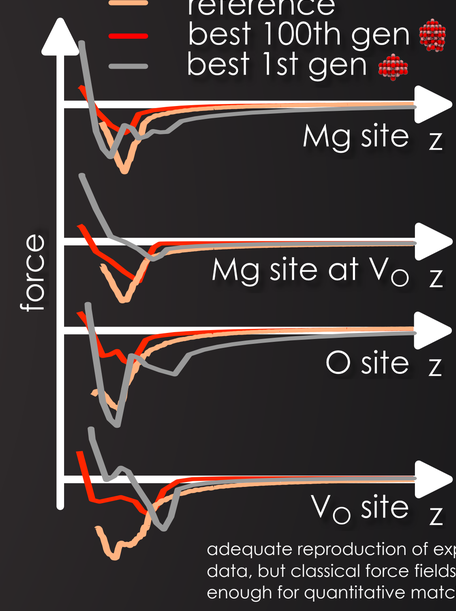
Ideal reference



perfect match, but not unique

Vs. experiments - MgO (100)

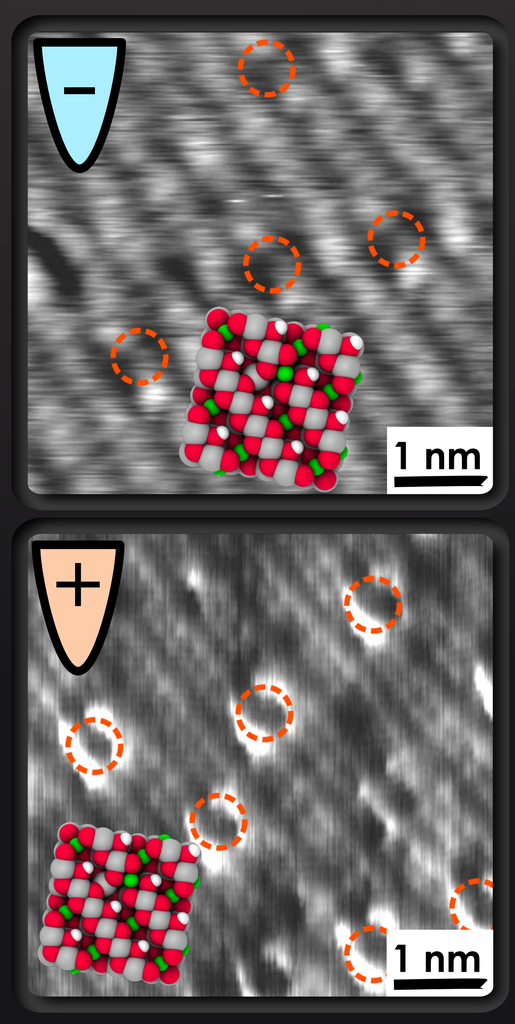




adequate reproduction of experimental data, but classical force fields not good enough for quantitative match

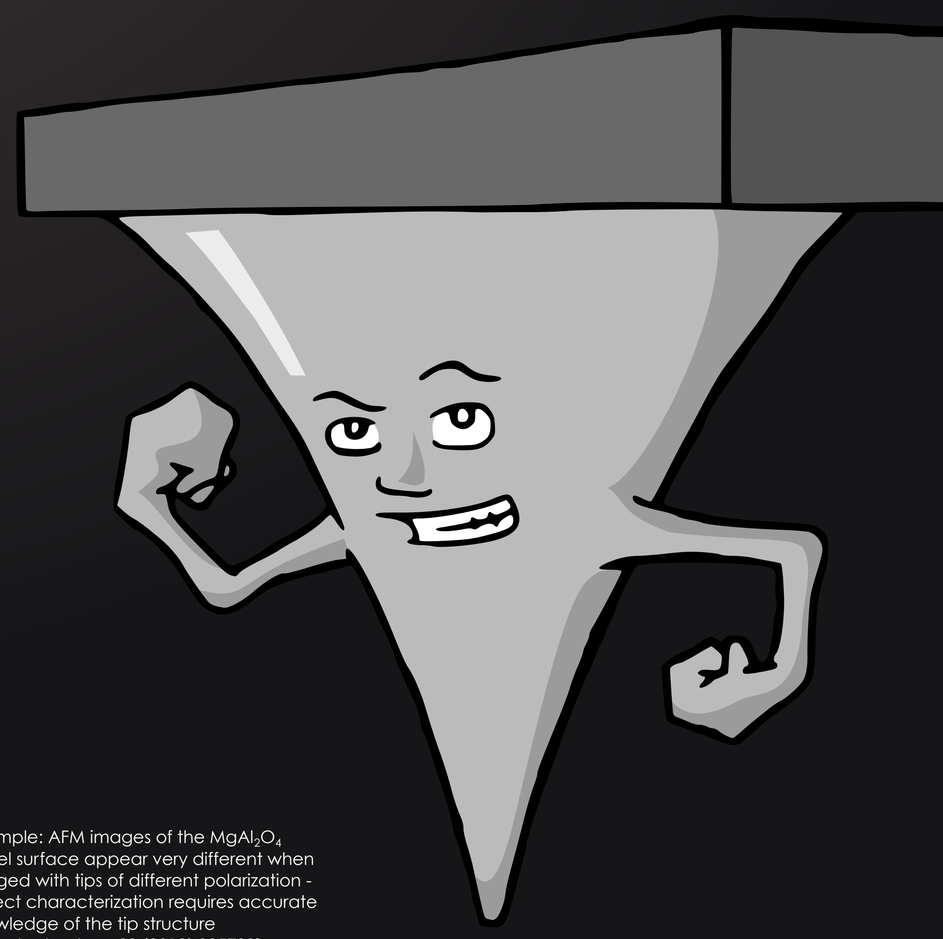
The atomic force microscope studies surfaces by feeling them with an atomically sharp tip

Different tips give different signals - *what do we see?*



example: AFM images of the $MgAl_2O_4$ spinel surface appear very different when imaged with tips of different polarization - defect characterization requires accurate knowledge of the tip structure [Nanotechnology **23** (2012) 325703]

A "reflection" of the tip in the images - *what is the tip?*



Good news

- good qualitative estimates
- good sampling of configuration space
- multiple solutions
- tip structure constrained by boundary structure
- metastable structures appear
- classical potentials not enough, needs ab initio

Bad news

- ab initio still too expensive