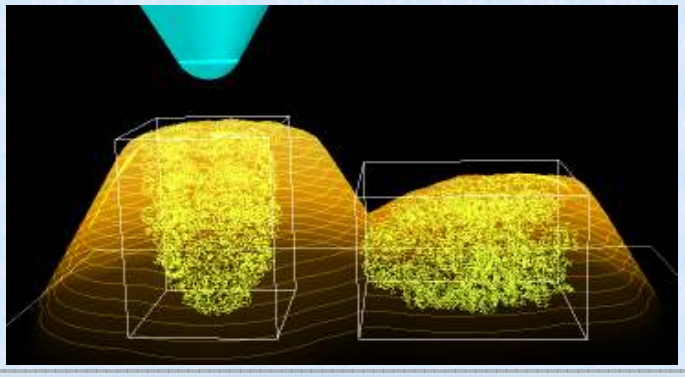
Advanced simulator for the SPM

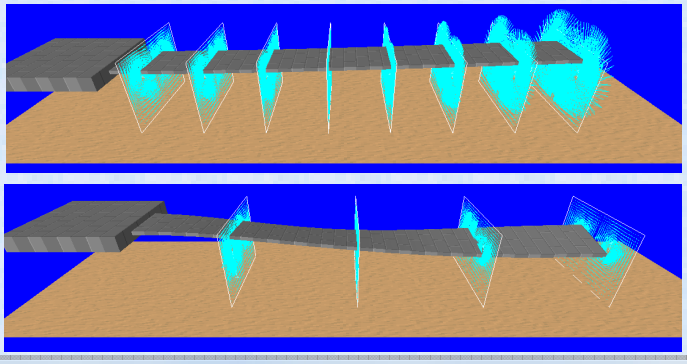
1. Geometrical Mutual AFM Simulator

・Estimate, within a second , one unknown item of 1)AFM image, 2)sample shape, or 3)tip shape based on the remaining two known items.

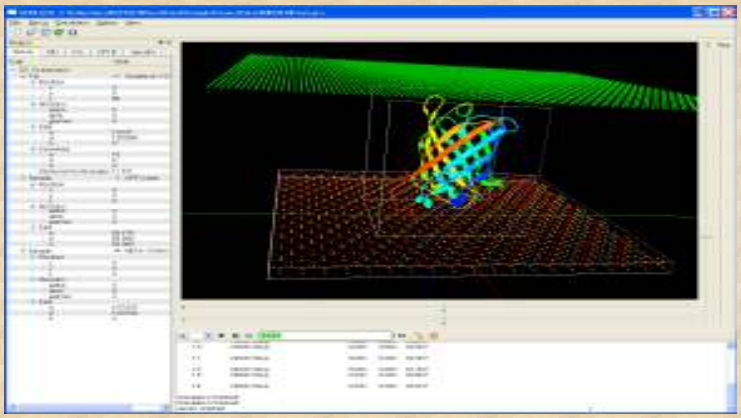


2. Soft Material Liquid AFM Simulator

・Simulate bending /twisting oscillation of a cantilever in liquid near the sample.
・Predict the tapping/dynamic mode AFM observables on soft materials in liquids.



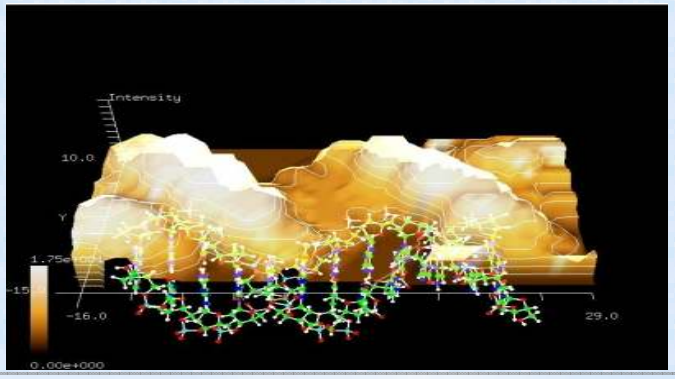
Integrated GUI software



・Provide a common platform for our SPM simulators.
・Manage and integrate tip/samples data, setup conditions and simulation results.

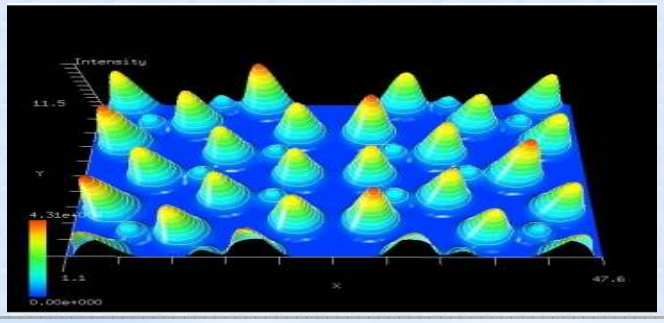
3. Classical Force Field AFM Simulator

・Calculate AFM images by the energy relaxation and the molecular dynamics method.
・Simulate AFM images for the dynamic AFM in liquids.



4. Quantum Dynamics SPM Simulator

・Based on the electronic state of the system, calculate AFM and STM/KPFM images and spectra.
・Adopt Density Functional based Tight Binding method , and perform much faster calculation than Density-funvtional-theory.



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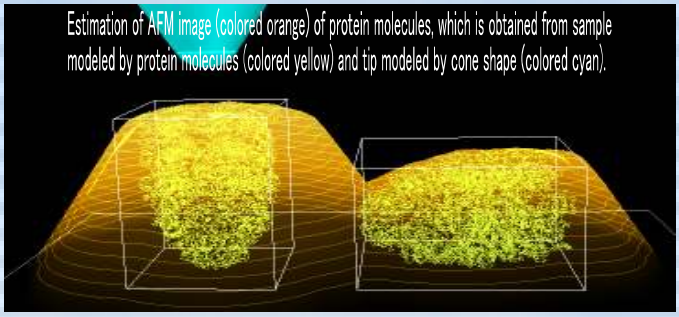
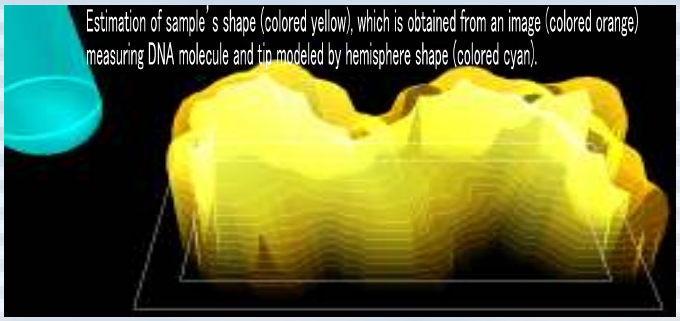
This development was supported by SENTAN, JST.

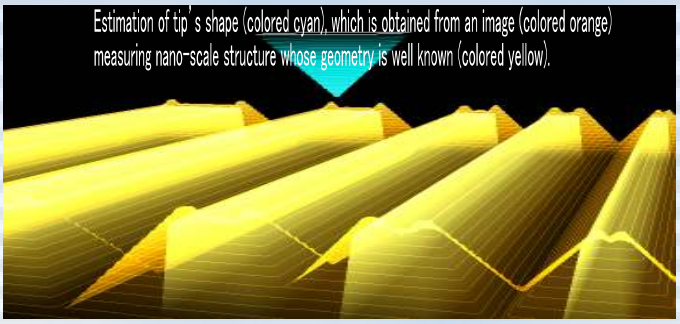
Advanced simulator for the SPM

1. Geometrical Mutual AFM Simulator

- This software estimates the image of AFM, shape of the sample, and shape of the tip respectively within a second using geometrical method.
- The geometrical method utilized in this software converts both atomic structure of the tip and sample proteins into grid surface models, and calculates contact height of the tip with the sample as an approximation of the image of AFM. Due to this geometrical method, this software can complete calculations within a second.
- Using a similar method for images measured by AFM and modeled structure of the tip, this software also estimates the refined shape of the sample.
- Besides, this software estimates the shape of the tip attached on the AFM device from images measured by AFM and samples whose geometrical structure are known.
- These mutual simulations among image, sample and tip could support SPM users from many aspects.

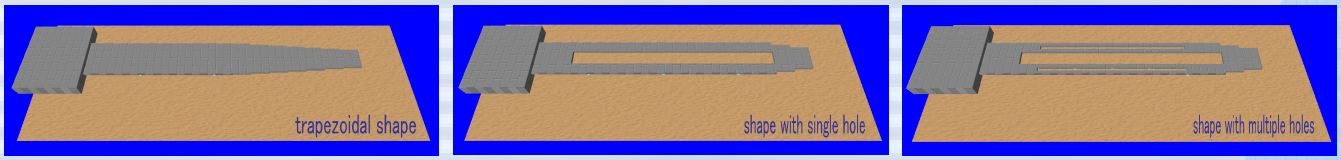




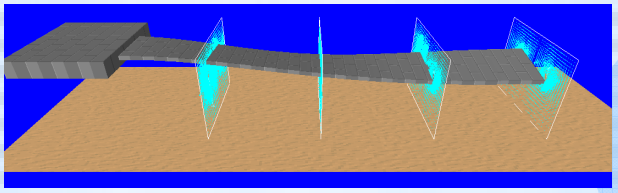


2. Soft Material Liquid AFM Simulator

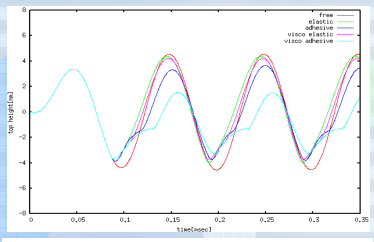
- This software calculates bending and twisting oscillation of an elastic cantilever, embedded in liquid, tapping its tip on soft material samples.
- This software calculates both the elastic dynamics of the cantilever and fluid dynamics around the cantilever simultaneously.
- Many aspects of cantilever motion in liquid can be estimated by this software. For example, the resonance frequency of the cantilever designed to work in vacuum, and how it changes in liquid, or by tapping soft material samples.



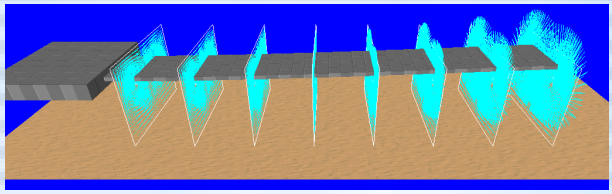
Complicated cantilever structures, trapezoidal shape, shape with single hole, and shape with multiple holes.



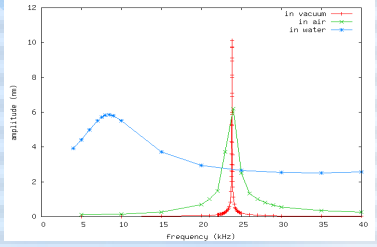
Elastic bending oscillation of the cantilever in liquid (drawn emphatically)



Time-evolution of the cantilever's head. These simulations are performed under several conditions, 1) free motion, 2) tapping an elastic material with the tip, 3) tapping adhesive material, 4) tapping viscous elastic material, and 5) tapping viscous adhesive material.



Elastic twisting oscillation of the cantilever in liquid (drawn emphatically)



Frequency spectrum of the cantilever head. These results are obtained using some conditions of fluid material around the cantilever, 1) vacuum, 2) air, and 3) water.

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Advanced simulator for the SPM

3. Classical Force Field AFM Simulator

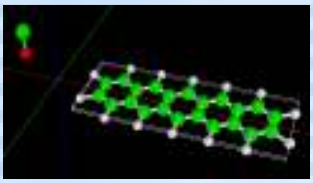
3-1. Energy relaxation method

This solver calculates the most stable atomic structure on the classical force field potential and the force that the probe received from the sample by the conjugate gradient (CG) method.

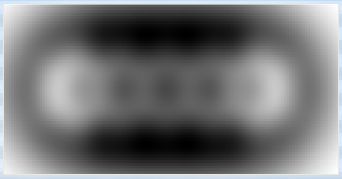
Example of NC-AFM simulation

We calculate the frequency shift image of pentacene by using CO probe in constant-height mode.

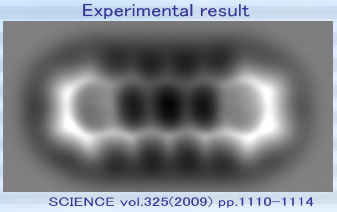
Ball-and-stick model of the pentacene molecule and the CO-probe.



Simulation result



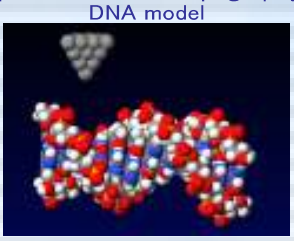
Experimental result



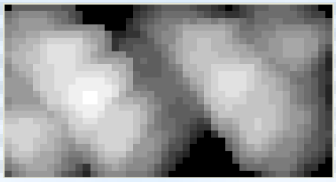
SCIENCE vol.325(2009) pp.1110-1114

Example of NC-AFM topography image

DNA model



Simulation result

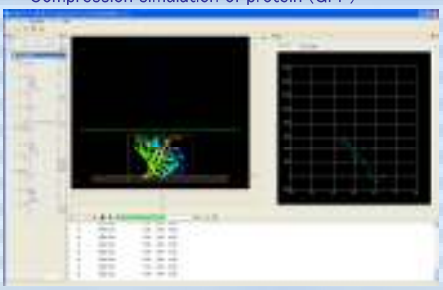


3-2. Molecular dynamics method

Calculating the AFM tip-substrate interaction is performed by molecular dynamics simulation method (MD). In this method, equations of motion of all the atoms in the simulation system are solved, and resulting the force curve and the trajectory of atoms are obtained.

Example of calculating Force curve

Compression simulation of protein (GFP)

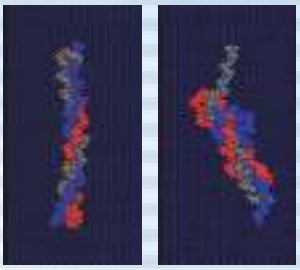


Our simulator will be able to make you observe the force curve and the corresponding deformation behavior of molecules.

Example of AFM imaging simulation

AFM imaging of collagen adsorbed to the HOPG substrate

Molecular model

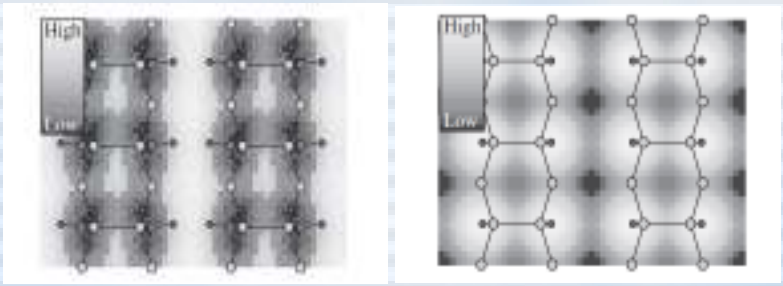


Simulation result

Katsunori Tagami and Masaru Tsukada, e-J. Surf. Sci. Nanotech. Vol. 4 (2006) 294-298.

4. Quantum Dynamics SPM Simulator

ncAFM topography (Masago et al. 2009)
H-Si(001) and CH_3-Si(001) surfaces



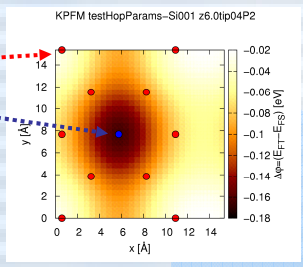
A cavity-like region is observed around the adsorbed methyl radicals despite of its protrusion (left). In the case of the H-terminated surface (right), a protrusion is observed on the H-adsorbed site.

KPFM : one dopant in Si(001)-c(4x2) surface
4.2 Å below the top

Map patterns change drastically!

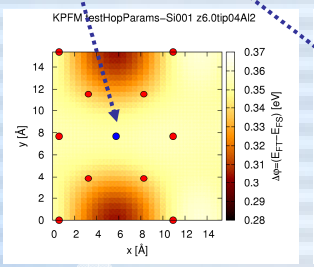
Si (up dimer)

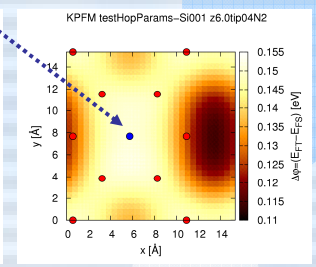
Phosphorus



Aluminum

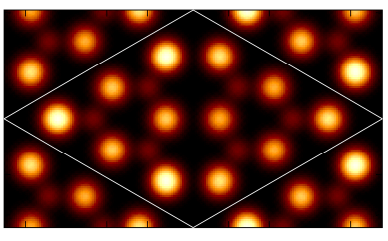
Nitrogen



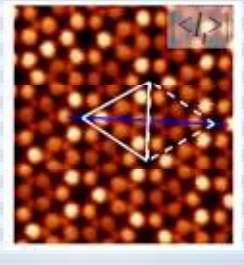


STM : Si(111) DAS 7x7 model

Sim.

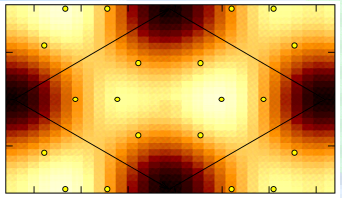


Exp. by Sawada et al. (2009)



Our simulation (left) reproduces the contrast of the spots in faulted and unfaulted half-unit cells measured by the experiment (right).

KPFM : Si(111) DAS 5x5 model



Local contact potential difference is larger around the adatoms and the rest atoms, though smaller around the corner holes.

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