Advanced Simulator for Scanning Probe Microscopy

Japan Science and Technology Agency

**Development of System and Technology for Advanced Measurement and Analysis
"Scanning Probe Microscopy Simulator"**

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Contact information

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aas ADVANCED ALGORITHM & SYSTEMS

Seminar information

Luncheon Seminar
        - Introduction to SPM Simulator -
2011.12.14 (Wed.)   12:05 – 12:55
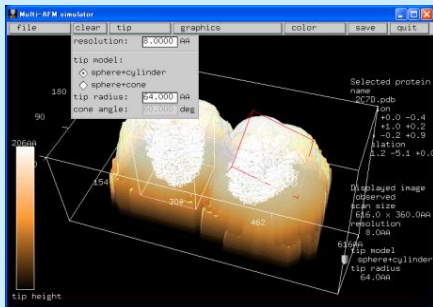**Room-A(Tôgen), 2F, Tower Hall Funabori**

*The 6th International Symposium on Surface Science
December 11-15,2011   Tower Hall Funabori – Funabori, Tokyo, Japan*

wpi
World Premier International
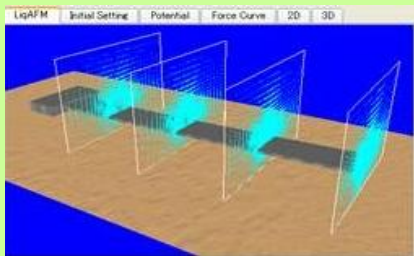Research Center Initiative

Outline of SPM Simulators

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.
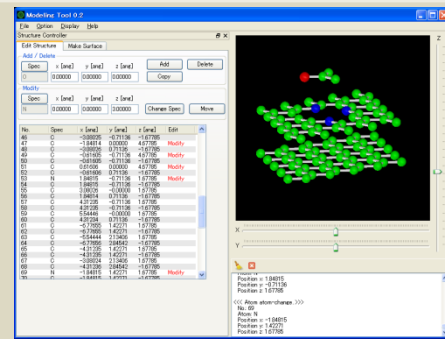

Modeling Tool

✓ Atomic structures can be built from the space group information.
✓ These structures can be modified for buliding advanced structures.

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.

Integrated GUI software

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

2. Soft Material Liquid AFM Simulator

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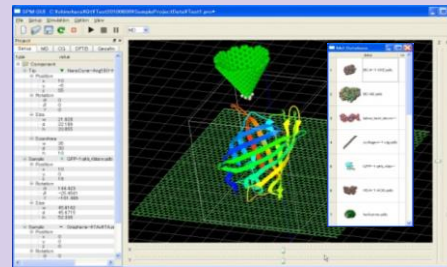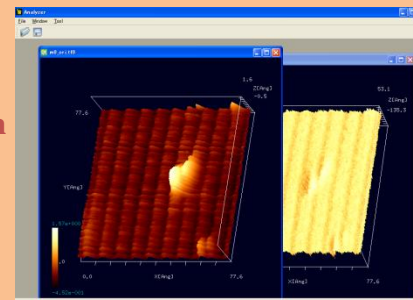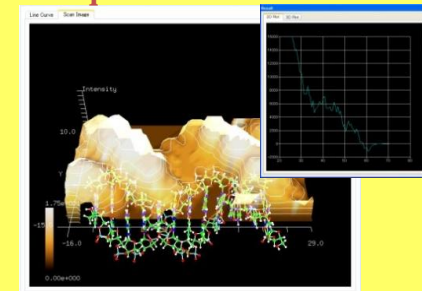✓ Predict the tapping/dynamic mode AFM observables on soft materials in liquids.


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-functional-theory.

Experimental Data Processing

✓ Powerful Image Visualization Module with Easy Handling.
✓ Function for Converting Various Data Formats.

[Offered from Fukutani Lab., IIS, Tokyo University]

1. GEOMETRICAL MUTUAL AFM SIMULATOR
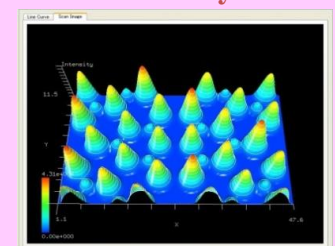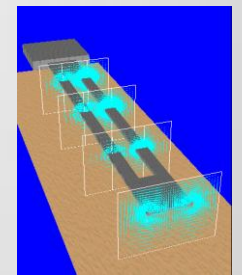
2. Soft Material Liquid AFM Simulator

Rapid calculation of AFM images by geometrical condition with meso-scale resolution

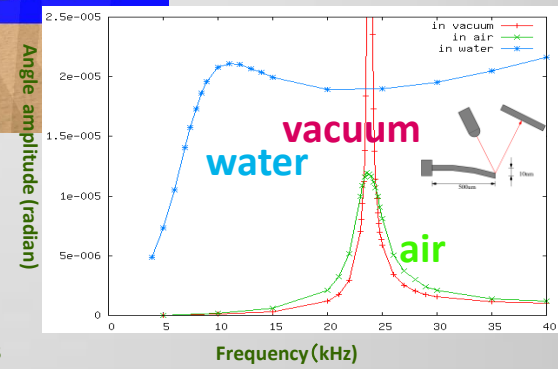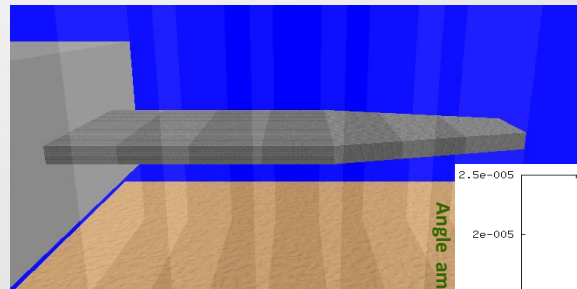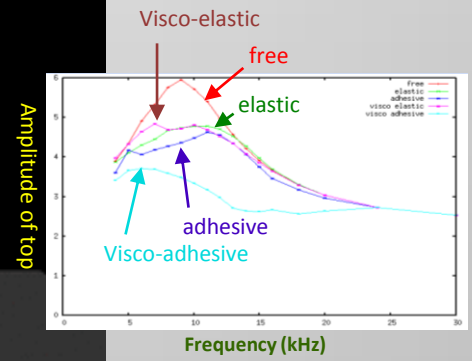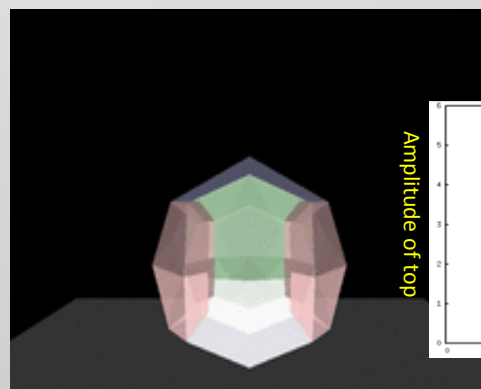Correction to large deformation of the tip/sample by classical mechanical method
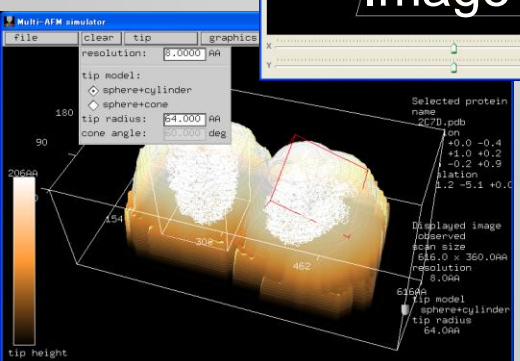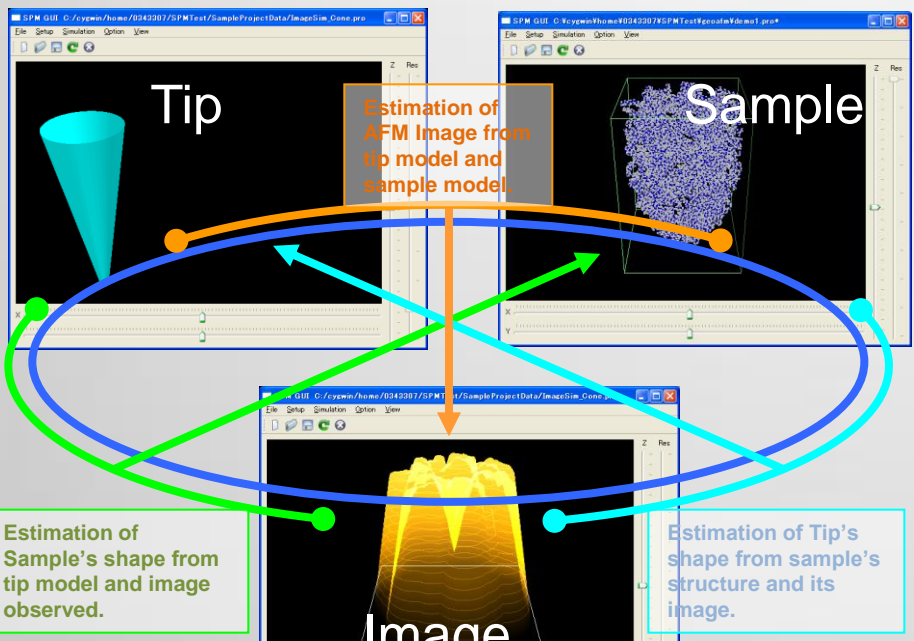
Oscillation analyses of cantilever in liquids, and dynamic AFM analyses of visco-elastic samples in liquids can be performed

Tip

Sample

Estimation of AFM Image from tip model and sample model.

Image

Estimation of Sample's shape from tip model and image observed.

Estimation of Tip's shape from sample's structure and its image.

Resonant curves of Si beam cantilever in water

Angle amplitude (radian)

vacuum

water

air

Frequency (kHz)

Resonant curves for tapping modes

Visco-elastic

free

elastic

adhesive

Visco-adhesive

Amplitude of top
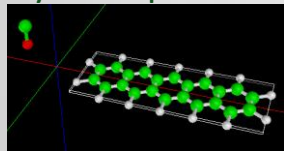
Frequency (kHz)

3. CLASSICAL FORCE FIELD AFM SIMULATOR
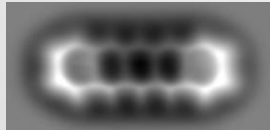
AFM image simulations by classical MM/MD
  MM: Molecular Mechanics
  MD: Molecular dynamics

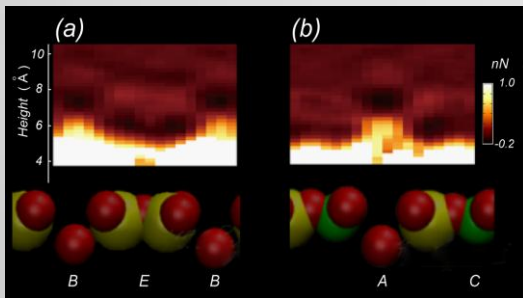## -examples-

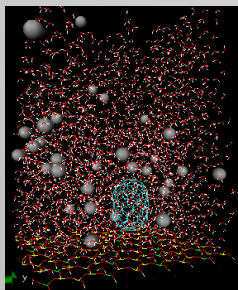**AFM image of pentacene by the CO tip**

Simulation
（calc. time on PC 20 min）

Experiment
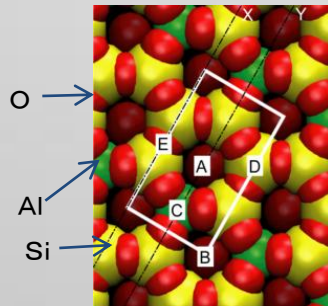L.Gross, F.Mohn, N.Moll, P.Lilijeroth, G.Meyer, SCIENCE, 325 (2009)1110

Simulation for dynamic AFM image of mica in water

(a)   (b)

Height (Å)
nN
1.0
-0.2

B   E   B   A   C

A snap shot of MD

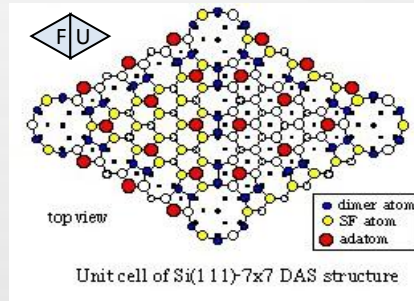**Model of mica in water**

O
Al
Si

E   A   D
C   B

4. Quantum Dynamics SPM Simulator
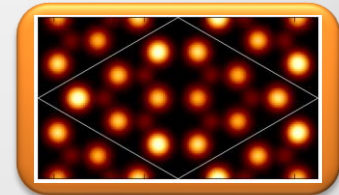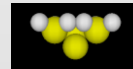
Accurate SPM image simulation by the quantum mechanical calculation

-examples-

STM image of Si(111)-7x7 DAS surface

F | U

top view

- dimer atom
- SF atom
- adatom

Unit cell of Si(111)-7x7 DAS structure

Tip model Si$_4$H$_9$

Simulation
（calc. time on PC 1.5 hour）
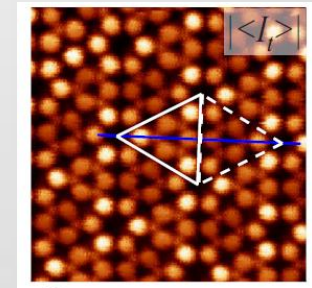
Experiment
by Sawada et al. (2009)

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KPFM (V$_{LCPD}$) images of H-Si(100) based surfaces
- PR-DFTB method was used -

H-Si(100)   Vacancy/H-Si(100)   Si (100) c(4X2)

Substituted by N

by P

by Al