Advanced Technology and Information Science

SPM (Scanning Probe Microscopy) Simulator catalog: fundamental

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We issue this catalog thanks to instructions given by Professor Masaru Tsukada, the Advanced Institute for Materials Research (AIMR) at Tohoku University, and many other researchers of the SPM. We plan to sell SPM Simulator from September 2014.

AASRI
Advanced Algorithm & Systems

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Guides for users

- Video tutorials for explaining how to carry out simulations

  We provide captured video files of carrying out various simulations for users who will use SPM Simulator from now on. You can access these files from the URL below.

  http://www.aasri.jp/pub/spm/en/SPM_movie_eng.html

  Watching these video files, you can easily learn how to operate typical sample calculations on the eight solvers in the SPM Simulator. (You can learn the operation procedures by cursor's movement such as clicking on an icon and mouse dragging.)

  Each sample calculation has operation movies (wmv format) indicating operation procedure, an operation procedure (excel format) describing how to operate in detail and an archive file (zip format) containing configuration and output files. By the use of these files, a beginner can use SPM Simulator easily.

  If you want to calculate a specific problem, you can carry out the simulation by selecting a sample calculation similar to the problem and editing the conditions on the setting file.

- A link for Guidebook of SPM Simulator

  In this brochure, we show examples of simulations. We also show each example’s corresponding solver included in SPM Simulator. You can refer to Guidebook of SPM Simulator for clarifying capabilities of solvers. From this information, you can estimate a price for solvers you need. You can access SPM HP (home page of SPM Simulator) without a password from here.

SPM Simulator

Unification of theoretical simulations and experiments: Scanning Probe Microscope

From laboratory of university in Japan, as de facto standard

What is SPM (Scanning Probe Microscope) Simulator?

- It carries out numerical simulations for various SPM experiments.
- It performs simulations according to the continuum mechanics, the fluid dynamics, the molecular dynamics method and the density functional theory.
- It can apply various digital image processing techniques to experimental SPM images.
- It can derive new knowledge from comparisons between experimental data and simulation results.

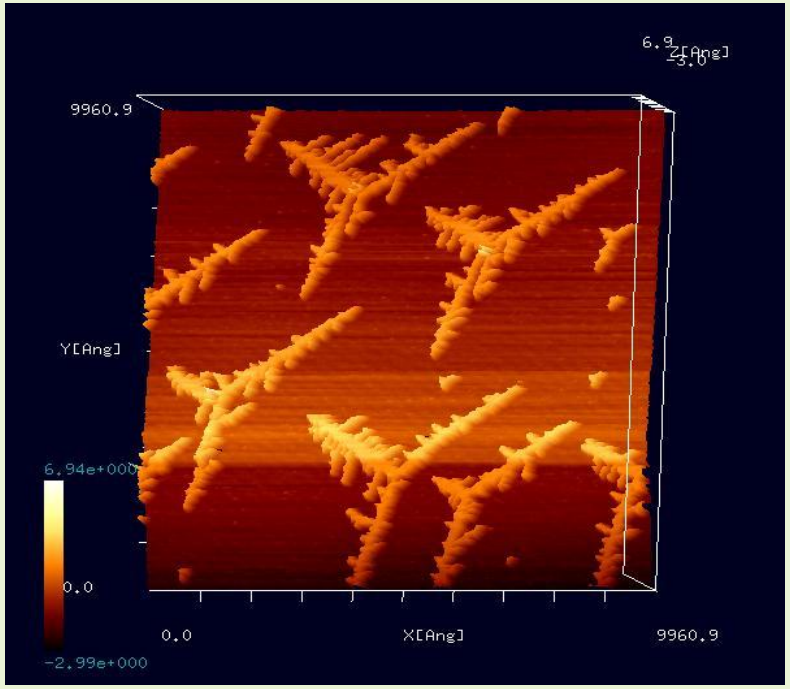
SPM Simulator can process both the experimental SPM images and images obtained as numerical simulation results in the same platform. Because of this characteristic, SPM Simulator is totally new and unique software all over the world.

A range of applications

●From conventional surface science (surface physics and surface chemistry) to biological surface science, researchers in various fields can enjoy SPM Simulator.

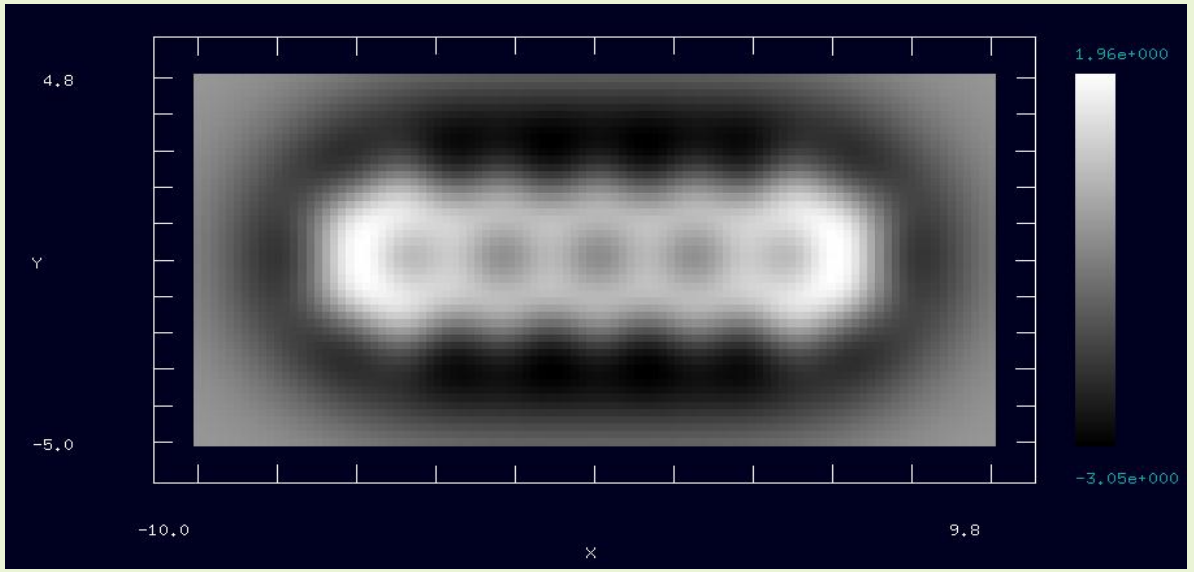
●From analyses of surfaces of metals and semiconductors, chemical reactions in catalysts, to imaging DNA and other biomaterials, SPM Simulator suits many different needs in a wide range of research activities.

●In future, we hope that SPM Simulator is utilized in the factories of nanoscale devices.

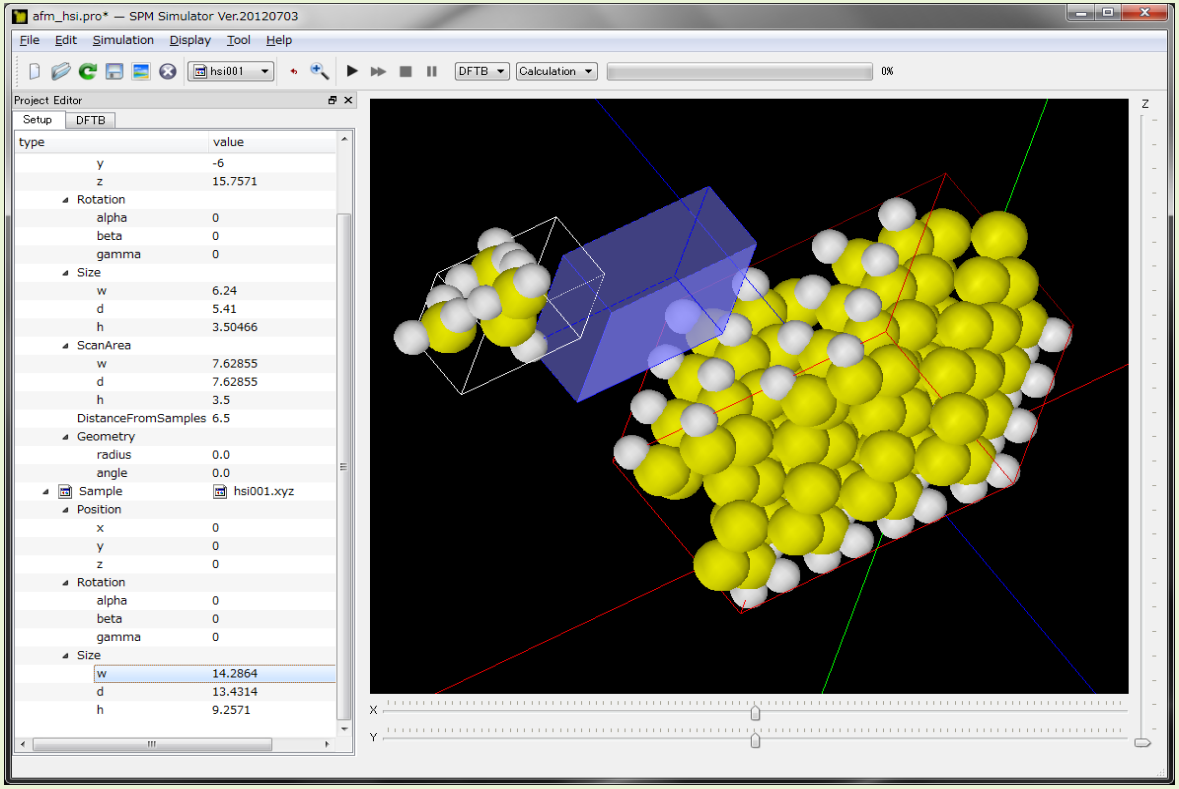


Impressive representation of experimental SPM images

[This image date is provided by the laboratory of the Professor Fukutani, Institute of Industrial Science, the University of Tokyo. It is obtained by depositing Au atoms on an Ir substrate and annealing them. Au islands form on the Ir substrate in a way of self-organization. S. Ogura et al., Phys. Rev. B **73**, 125442 (2006); S. Ogura and K. Fukutani, J. Phys.: Condens. Matter **21** (2009) 474210.]

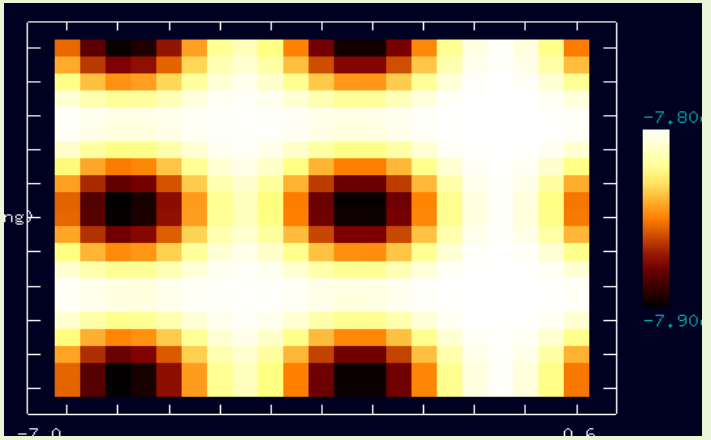


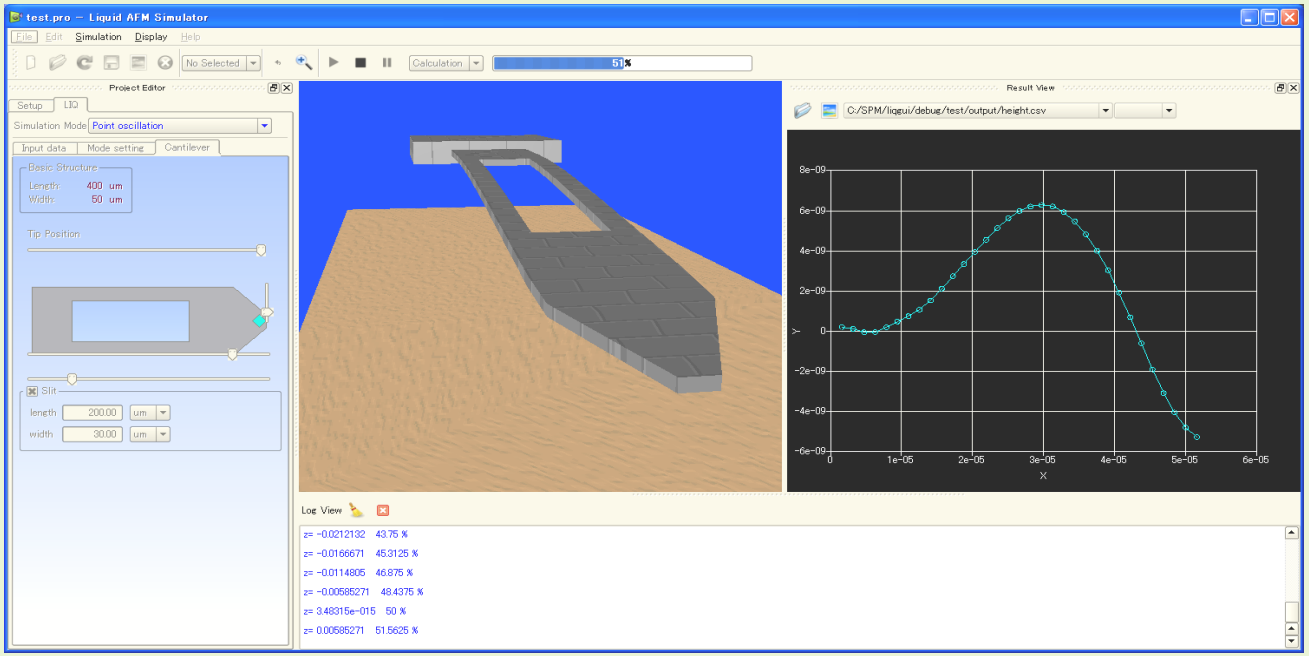
A frequency-shift AFM image of a molecule of pentacene obtained by geometry optimizing AFM image Simulator (CG)



A frequency-shift AFM simulation with DFTB solver. In the simulation, we scan the hydrogenated Si(001) surface with the modeled Si tip apex hydrogenated.

An obtained frequency-shift AFM image. In this image, hydrogen atoms are represented as black circles.





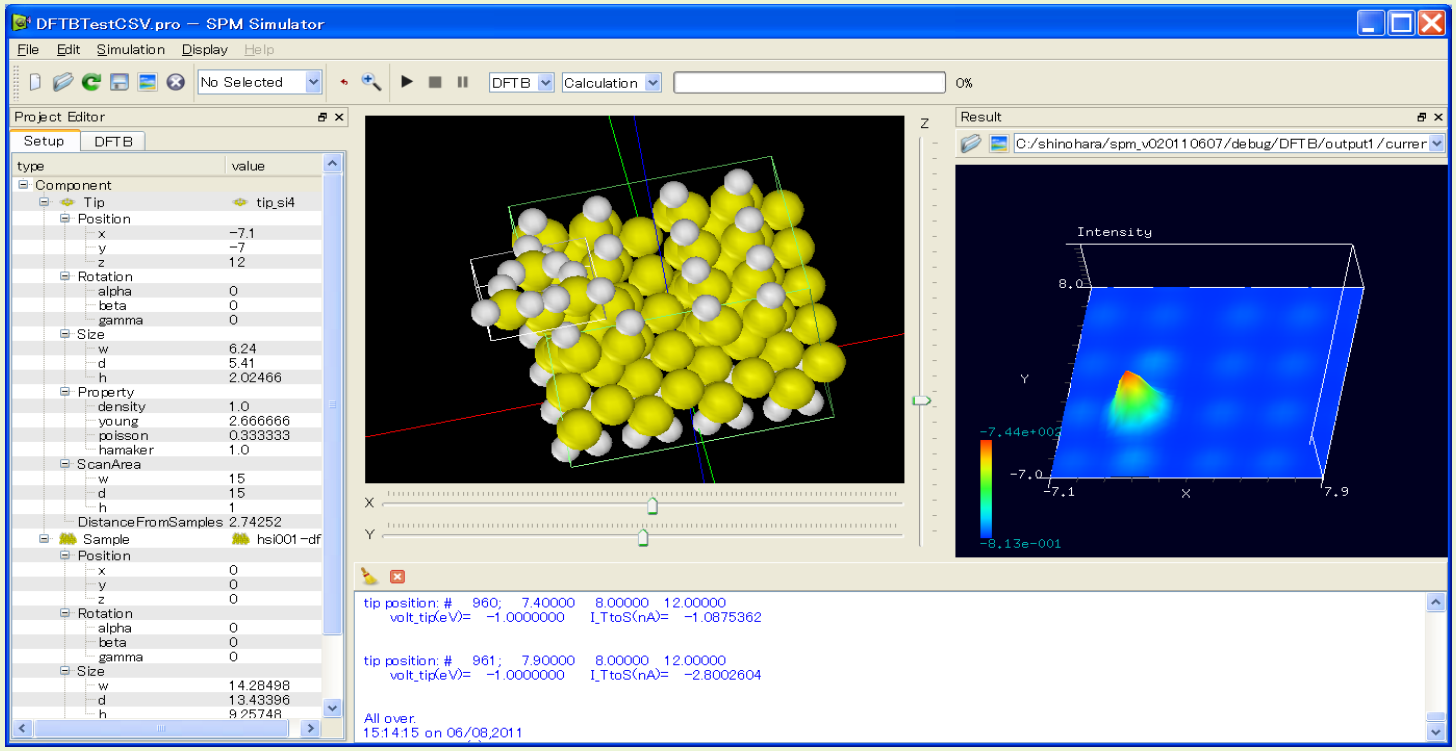
GUI for the simulation of AFM in liquid environment. In this simulation, movement of the cantilever is examined.

Differences between conventional software and our SPM Simulator

- Using SPM Simulator, researchers, who are not familiar to theoretical physics precisely, can perform numerical simulations with ease.
- Because of the superior and user-friendly GUI, you can carry out simulations efficiently.
- Because of rational project management, you can verify the history of simulations and save their data properly.

SPM Simulator is user-friendly

Because of the highly refined GUI, researchers, who are not familiar to theoretical physics precisely, can perform various simulations of the Scanning Probe Microscopy with ease.

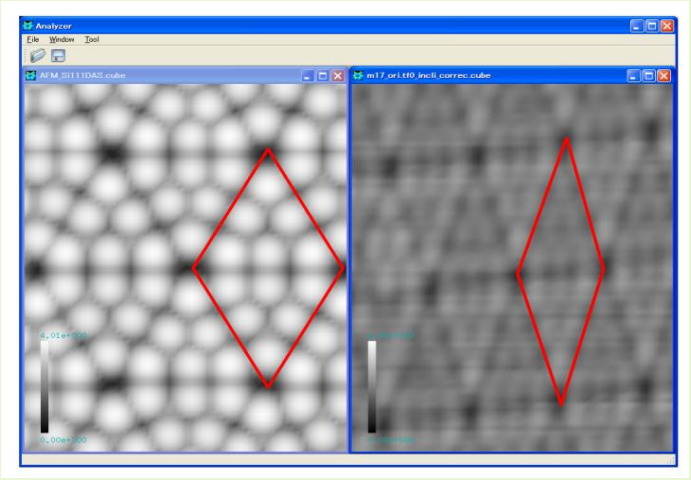


An example of the GUI

Various convenient tools for beginners

SPM Simulator offers the unique and de facto standard simulation for the SPM: unification of experiments and theoretical simulations.

Bundling SPM Simulators with SPM instruments supplied by makers all over the world, simulations of the SPM become popular. This activity will cause advances of the technology in the field of SPM.



In the SPM Simulator, the solver Analyzer (a digital image processor for experimental SPM data) is equipped.
http://www.aasri.jp/pub/spm/pdf/SPM_guidebook/Analyzer_eng.pdf
The solver Analyzer can import experimental binary data, which are output from SPM instruments of various makers. The Analyzer supports many file formats for various instrument type.

Moreover, the Analyzer has advanced digital image processing tools, so that you can analyze experimental SPM data with ease.

As mentioned above, the SPM Simulator is a very comprehensive software. It can be bundled with any SPM instrument supplied by any maker all over the world.

Experimental SPM images are often difficult to interpret and understand.

→ Referring to results of theoretical simulations are important.

SPM Simulator realizes the following three functions on the same platform.

[1] Theoretical and numerical simulation tools

Density Functional based Tight Binding (DFTB) method

→ Precise simulations of STM images and frequency-shift AFM images

[2] Digital image processing tools for experimental SPM data

SPM Simulator supports file formats for various instrument types, Omicron, Asylum, Bruker, and so on.

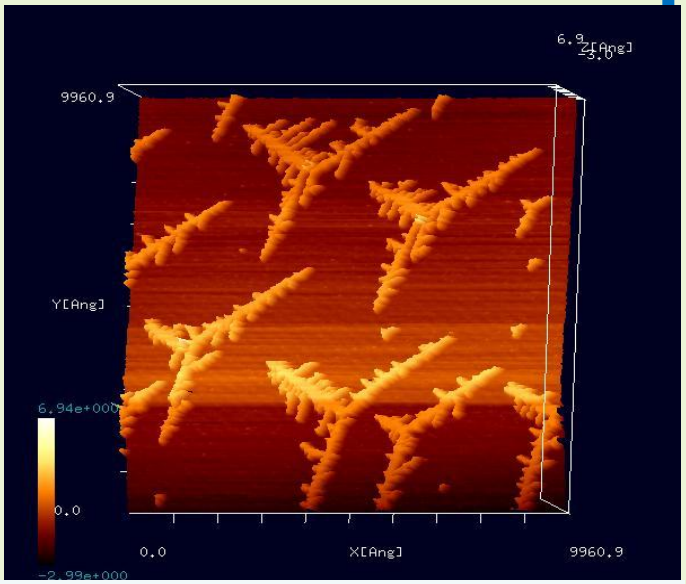
→ Importing experimental binary data in direct.

Blind Tip Reconstruction Algorithm,

Fourier analysis, etc.

[3] Tools for comparing theoretical simulation results and experimental SPM images

→ With various digital image processing tools, users can evaluate physical parameters by themselves.



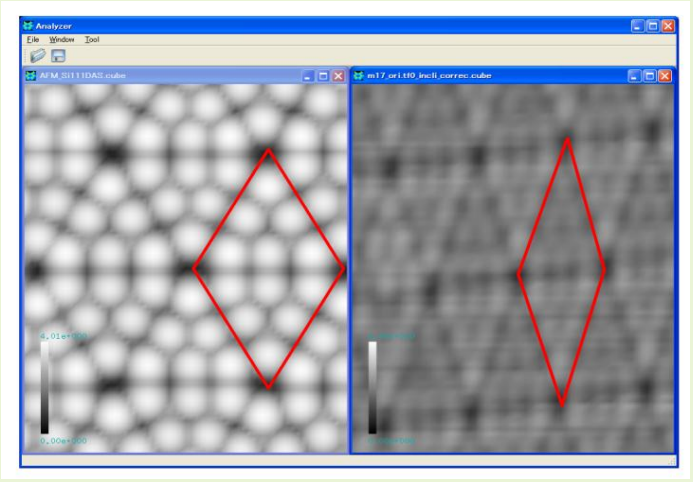
[This image date is provided by the laboratory of the Professor Fukutani, Institute of Industrial Science, the University of Tokyo.]

SPM Simulator offers the unique and de facto standard simulation for the SPM: unification of experiments and theoretical simulations.

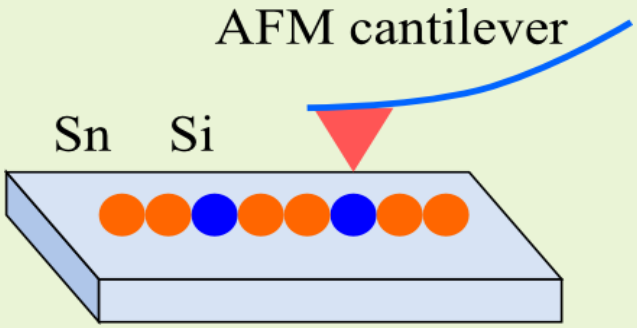
With the de facto standard of SPM Simulator all over the world, we hope that the SPM instruments will be used in factories of nanoscale devices.

⇒ In the factories, SPM instruments will be utilized not only for inspection equipments but also manufacturing equipments.

Using SPM instruments, we can produce nanostructures out of molecules and atoms.



AFM images of silicon wafers: a simulation result (left) and experimental image (right).
[This image date is provided by the laboratory of the Professor Fukutani, Institute of Industrial Science, the University of Tokyo.]



Producing a nanostructure out of atoms with an AFM instrument.

SPM (Scanning Probe Microscopy) Simulator: A chart of needs, fields of applications and suitable solvers

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
The tip shape estimation	The Blind Tip Reconstruction Method	General surface science	Analyzer	Because we have to estimate a shape of the tip from the experimental data of SPM, we can regard it as an inverse problem that has infinite number of solutions, that is to say, infinitely many possible shapes for the tip. With the solver Analyzer , we can choose a preferable shape of the tip by specifying some parameters.
	Removing artifacts from the experimental image data of the SPM.	General surface science	GeoAFM	Using the solver GeoAFM, we can save the data of the estimated shape of the tip as a text file. Combining this data of the tip and an experimental image data of the SPM together, we can obtain an original image of the sample surface.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
The tip shape estimation	Estimation of the original sample surface by applying the learning algorithm of the neural network to the experimental image data of the SPM.	General surface science	Analyzer	With the solver Analyzer, in order to examine the shape and other properties of the tip, we can apply the learning algorithm of the neural network to the experimental image data of the SPM. Using this machine learning method, we can construct the original image of the sample surface from other experimental image data obtained with the same tip.
	Calibration of the tip using a standard testing sample with steps	General surface science	GeoAFM	With the solver GeoAFM, we can obtain a shape of the tip rapidly from experimental image data of the standard testing sample and other sample surfaces.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Estimation of the amplitude of the cantilever oscillation for the AFM	Using the force-distance curve obtained from experimental data, we can evaluate the amplitude of the cantilever oscillation with calibration of piezoelectric positioning actuators. I want to compare this evaluated amplitude with results of the simulation.	Nanomaterials, chemistry, pharmacy, bioscience	LiqAFM	Using the solver LiqAFM, from the analysis of the cantilever oscillation, we can compute its amplitude.
Automatic estimation of structural parameters of the sample surface	Compensation of the tilt for the experimental image data of the sample surface	General surface science	Analyzer	We have already implemented a function for the compensation of the tile of the sample surface in the solver Analyzer.
	I want to create the 3D-xyz data of the structure of the sample surface.	General surface science	Analyzer, GeoAFM	Using the solvers, Analyzer and GeoAFM, we can store the 3D data of the sample surface obtained with an experiment as an original intrinsic data format (.cube).

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Automatic estimation of structural parameters of the sample surface	We want to examine the lengths of the edges of a unit cell and the angles between them in the lattice found on the experimental image data. Moreover, we want to view a cross section of the sample surface.	Inorganic materials, alloys, inorganic semiconductors, organic semiconductors	Analyzer	Using the solver Analyzer, on the image of the SPM experiment displayed in the monitor, we can specify two points with the mouse and obtain the length and the cross section between them. Furthermore, by specifying three points, we can measure the angle of a triangle defined with these three points.
Importing experimental data created by various SPM equipments of various instrument makers all over the world	We want to carry out the visualization of experimental binary data created by various SPM equipments of various instrument makers all over the world.	General surface science	Analyzer	The solver Analyzer supports the file format of the binary data for Unisoku, Omicron, Asylum, JEOL, Agilent, Shimadzu, and other major instrument makers.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Various shapes and sizes of cantilevers	I want to examine structural properties of cantilevers in various shapes and sizes, for example, a cantilever with many holes.	Nanomaterials, chemistry, pharmacy, bioscience	LiqAFM	The solver LiqAFM has functions to specify various shapes and sizes for the cantilevers.
Dissipation of the energy from the cantilever	I want to examine the dissipation of the energy caused by the interaction between the tip and the sample.	Nanomaterials, chemistry, pharmacy, bioscience	FemAFM, CG, DFTB	The solvers, FemAFM, CG and DFTB, can simulate the phase-shift AFM images, which provide information of the energy dissipation to us.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Digital image processing for experimental image data of the SPM	We want to apply the following digital processing to the experimental image data: •The 3D visualization •The contrast adjustment in a nonlinear manner •Removal of noises •Extracting edges •Carrying out the Fourier transformation of a 2D image and filtering certain frequency components	General surface science	Analyzer	The solver Analyzer has many powerful digital processing tools, and you can utilize them to gain deeper understanding of the experimental image data.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of the KPFM	I want to examine a distribution of positions of dopants on the surface of semiconductor. I want to examine a distribution of depths of them, as well. Moreover, I want to investigate quantum mechanical states of electrons on the surface of the sample.	Inorganic semiconductors, organic semiconductors	DFTB	We can simulate the KPFM with the solver DFTB.
	I want to simulate the AFM and the KPFM simultaneously.	Inorganic semiconductors, organic semiconductors	DFTB	Using the solver DFTB, we can simulate the phase-shift AFM image and the KPFM image simultaneously.
Advanced tools for constructing atomic crystalline and molecular models	I want to choose preferable atoms and construct crystalline and molecular models out of them in order to use them as samples of the SPM simulation.	Inorganic semiconductors, alloys, general inorganic materials	SetModel	Using the solver SetModel, we can construct crystalline and molecular models out of preferable atoms at ease.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Advanced tools for constructing atomic crystalline and molecular models	I want to choose preferable atoms and construct models of the tip out of them for using them in the SPM simulation.	Inorganic semiconductors, alloys, general inorganic materials	SetModel	With the solver SetModel, we can construct the atomic model of the tip at ease.
Simulation of the AFM images of macro-molecules, for example, proteins and DNAs.	Obtaining structural data of proteins from the Protein Data Bank, I want to simulate their AFM images.	Nanomaterials, chemistry, pharmacy, bioscience	GeoAFM, FemAFM	The solvers, GeoAFM and FemAFM, can import the data obtained from the Protein Data Bank in direct, and carry out the AFM simulation using them as samples.
Simulation of the viscoelasticity of the sample surface	I want to obtain the force-distance curve derived according to the viscoelasticity between the tip and the sample in air.	Nanomaterials, chemistry, pharmacy, bioscience	FemAFM	The solver FemAFM can simulate the contact mechanics between the tip and the sample according to the viscoelasticity specified with the surface tension and the cohesive force of the sample surface in air.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of the viscoelasticity of the sample surface	I want to obtain the force-distance curve derived according to the viscoelasticity between the tip and the sample in liquid.	Nanomaterials, chemistry, pharmacy, bioscience	LiqAFM	The solver LiqAFM can simulate the contact mechanics between the tip and the sample according to the viscoelasticity specified with the surface tension and the cohesive force of the sample surface in liquid.
Rapid simulation of the AFM images	I want to simulate not only the AFM images obtained by the experiments but also the images of the tip and the sample rapidly and conveniently, for example, the AFM images of the C60 layer with defects and other micro-particles deposited on substrates.	Nanomaterials, general inorganic materials, chemistry, pharmacy, bioscience	GeoAFM	Using the solver GeoAFM, we can simulate the AFM images obtained by the experiments and images of the tip and the sample rapidly according to the geometrical method. Although the GeoAFM adopts the geometrical method and its results do not contain precise physical meanings, it generates images of molecules and atoms quite exactly. The GeoAFM has wide application range for materials of various sizes.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of deformation caused by the atomic force between the tip and the sample	I want to simulate AFM images with considering the effects of deformation caused by the van der Waals force between the tip and the sample.	Nanomaterials, chemistry, pharmacy, bioscience	FemAFM	The solver FemAFM can simulate the AFM images with considering the effects of deformation caused by the van der Waals force between the tip and the sample, for example, examining the surface of bio-based soft materials with the AFM tips.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of the AFM images with molecular geometry optimization	I want to simulate the AFM images with searching geometry of a molecule that corresponds to the minimum of the total energy. •The AFM images of porphyrins, phthalocyanines and other large molecules deposited on the substrates •The AFM images of the self-assembled monolayers of organic molecules and long chain polymers deposited on metal substrates	Inorganic semiconductors, organic semiconductors, organic polymers	CG	The solver CG searches geometry of a molecule that corresponds to the minimum of the total energy with the conjugate gradients method for classical force field and the molecular mechanics method. From this function, the CG can simulate the AFM experiments under the deformation of molecules caused by the interaction between the tip and the sample. (The CG just finds a stable structure and it cannot examine the time evolution of the system.)

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of the AFM images with the molecular mechanics method	I want to simulate the AFM images with examining the time evolution of the molecular structure. •The AFM image of the formic acid deposited on the surface of TiO2(110) •The AFM images of the self-assembled monolayers of organic molecules and long chain polymers deposited on metal substrates	Inorganic semiconductors, organic semiconductors, organic polymers	MD	The solver MD can examine the change of the molecular structure by the passage of time numerically according to the molecular mechanics method. Using this function, the MD simulates the time evolution of molecular structure caused by the interaction between the tip and the atom during the AFM experiments.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of the AFM images in liquid under optimizing geometry of a molecule that corresponds to the minimum of the total energy	I want to obtain the AFM images in liquid with considering a change of free energy caused by the interaction between the tip, the sample and the solvent (water). Searching geometry of a molecule that corresponds to the minimum of the total energy, I want to carry out the simulation of the AFM experiments. For example, I want to obtain the force-distance curve when the tip of carbon nanotube gets close to the graphene sheet in pure water.	Inorganic semiconductors, organic semiconductors, organic polymers	CG-RISM	The solver CG-RISM searches the geometry of a molecule that corresponds to the minimum of the total energy in liquid by the Reference Interaction Site Model (RISM) method. From this function, the CG-RISM can simulate the deformation of molecular structure caused by the interaction between the tip and the sample during the AFM experiments. (The CG just finds a stable structure and it cannot examine the time evolution of the system.)

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of the AFM images with the molecular mechanics method under the thermal effects	I want to carry out simulation of the AFM experiments with considering the time evolution of the molecular structure caused by thermal relaxation.	Inorganic semiconductors, organic semiconductors, organic polymers	MD	The solver MD can introduce the thermal effects into the velocities of atoms according to the principle of the statistical mechanics. From this function, the MD can compute the time evolution of the molecular structure and simulate the AFM experiments under the condition of the constant temperature.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Simulation of the phase-shift AFM images for the soft materials	I want to simulate AFM experiments for proteins, DNAs, and other soft materials. •Simulation of the phase-shift AFM images •Estimation of the absolute values of the phase shift •Confirming the relaxation of the kinetic energy of the cantilever and the energy transport into the sample	Nanomaterials, chemistry, pharmacy, bioscience	FemAFM, CG, DFTB	The solvers, FemAFM, CG, and DFTB, can simulate the phase-shift AFM images. The FemAFM is suitable for examining organic polymers whose typical length scale is on the order of micrometer. The CG is suitable for examining the organic molecules whose typical length scale is on the order of 10 angstrom. The DFTB is suitable for examining the small sample whose typical length scale is on the order of 1 angstrom. Users can select preferable solver according to the size of the sample.
Advanced simulator for STM and AFM	Simulation for STM and AFM image based on first principle calculation	Nanomaterial, electronics, surface science	DFTB	SPM images are simulated by calculation of a quantum-mechanical electronic states.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Advanced simulator for STM and AFM	To predict AFM, STM, STS and KPFM images in atomic resolution.	Nanomaterial, electronics, nano-device, quantum chemistry, surface physical property	DFTB	It is possible to calculate STM, STS, AFM and KPFM images by DFTB.
Simulation of the sample	Sample’s deformation and Sample’s dynamic reaction	Bioscience, organic chemistry	FemAFM, LiqAFM, MD	For calculation of continuous elastic body, such as biopolymers, FemAFM and LiqAFM is suitable. For calculation of a low molecule, such as octane, MD is suitable.
Holding angle of cantilever	Influence of tip’s angle	Bioscience	GeoAFM, FemAFM, CG, MD, DFTB	A tip's inclination can be set on GUI.
	Influence of cantilever angle in underwater measurement	Bioscience	LiqAFM	Vibration of cantilever underwater can be simulated in consideration of inclination of cantilever.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Surroundings of cantilever	Influence of temperature and humidity in atmosphere, and influence of kind of solution in liquid	Bioscience	LiqAFM	An atmospheric temperature, an atmospheric humidity or kind of solution can be set up by the density and viscosity of fluid.
AFM image of biomolecules	Simulation for collagen molecules	Bioscience, medical science, pharmacy	GeoAFM, FemAFM, CG, MD	GeoAFM is suitable for fast calculation. CG and MD is suitable for accurate calculation.
	Simulation for collagen fibril, chromosome, DNA, amyloid, microtubule and protein	Bioscience, medical science, pharmacy	GeoAFM, FemAFM	GeoAFM is suitable for simulation of a biological tissue with a large molecular weight. FemAFM is suitable for simulating a tissue precisely as an elastic body.
Properties of a highly polymerized compound	AFM image and force curve of a tire (rubber) and a polymer	Bioscience, organic material	GeoAFM, FemAFM, CG, MD	It is possible to calculate AFM image by each solver, viscoelastic contact analysis by FemAFM and force curve by CG and MD.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Properties of nanomaterial	Shape and hardness of CNT and graphene	Nanomaterial, organic material	CG, MD	It is possible to calculate an AFM image and a force curve. Force curve underwater also can be calculated by CG.
Samples condition and result	Immobilization states of a sample molecule on a substrate	Organic chemistry	CG, MD	Whether the atom is immobilized or not can be selected in CG and MD. Dynamics of a molecule can be simulated by MD.
A sample in liquid and a sample in the atmosphere	Analysis in liquid and in the atmosphere	Bioscience	LiqAFM, CG	It is possible to simulate vibrational analysis and viscoelastic analysis in liquid and in the atmosphere by LiqAFM. It is possible to simulate force curve in liquid by CG.
Image of a kelvin probe force microscopy	Prediction of a local contact potential difference image (LCPD image) of a semiconductor surface and metal surface in atomic resolution	Surface properties, nano device, nanoelectronics	DFTB	We have published papers on the calculation result of Si(001)-c(4x2), Si(001)-p(2x1):H and Si(111)-(5x5).

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Distribution of work function on the semiconductor surface	Local contact potential difference image on a semiconductor surface	Inorganic material, nano device, nanoelectronics	DFTB	Local contact potential difference on a doped N-type semiconductor and a doped P-type semiconductor can be calculated.
Surface structure of metal, semiconductor and so on	STM image on a metal surface and on a semiconductor surface	Onorganic material, nano device, nanoelecstonics	DFTB	STM image of a Si(001) surface, Au(001) surface, a molecule on a substrate, and so on, can be simulated.
	Frequency shift image on a semiconductor surface and on an insulator	Inorganic material, nano device	DFTB	It is possible to simulate AFM image on Si(001) surface and on TiO2(110) surface and so on.
Presumption of dopant's properties on semiconductor surface	Presumption of position, depth and element of the dopant by numeric calculation	Inorganic material, nano device, nanoelectronics, semiconductor	DFTB	STM image and KPFM image of doped silicon surface can be simulated.

Needs for simulation	Details of the needs	Fields of applications	Suitable solvers	comments
Presumption for properties of metal and semiconductor	Presumption of density of states on a semiconductor surface and a metal surface	Inorganic material, nano device, nanoelectronics	DFTB	It is possible to simulate scanning tunneling spectroscopy (STS) at the tip's set up position on the semiconductor surface and metal surface.
	Properties of material related to catalyst	Surface property, catalyst chemistry	DFTB	It is possible to simulate STS curve and KPFM image of catalytic metal surface such as platinum and ruthenium.

Composition of SPM Simulator

Analyzer	Digital image processor	
	The Analyzer loads the experimental binary data from SPM devices made by various companies. Advanced image processing. Comparison between the experimental image and the simulated image.	
GeoAFM	Geometrical Mutual AFM Simulator	Geometry
	Nanostructured semiconductor devices, polymers, bio-polymers	
FemAFM	Finite Element Method AFM Simulator	Classical theory
	Nanostructured semiconductor devices, polymers, bio-polymers	
LiqAFM	Soft Material Liquid AFM Simulator	Classical theory
	Polymers, biomolecules	
CG	Geometry Optimizing AFM Simulator	Classical theory
	Organic small molecules, inorganic materials	
MD	Molecular Dynamics AFM Simulator	Classical theory
	Organic small molecules, inorganic materials	
DFTB	Quantum Mechanical SPM Simulator	Quantum theory
	Frequency shift AFM, STM, KPFM images for nano-size structures	
SetModel	Atomic Structure Modeling Tool	
	Preparation of the atomic structure, e.g. the lattice structure	

Analyzer	Digital image processor	
Property	It performs the digital processing of the SPM experimental data and the simulated image data together.	
Capability	It can load the experimental binary data from SPM devices produced by various companies. Advanced digital image processing. The experimental image and the simulated image are displayed on the same window. The digital processing and the comparison of them gives us a new insight.	
Advantage to the conventional simulators	This is the only one software in the world to treat the experimental and the simulated data on the same platform.	
Application field	Inorganic/organic materials, nano-materials, organic soft materials, chemistry, pharmacy, bioscience	

GeoAFM	Geometrical Mutual AFM Simulator	Geometry
Property	Extremely high-speed AFM simulation. It is suitable for micron-size sample. It can simulate AFM images for proteins, DNA etc. in liquid.	
Computing method and target	It provides users with a kind of a three-way data processor; it can reconstruct the one out of the other two among three geometrical elements, a tip, sample material and its AFM image. It shows a greatest performance especially for a large material such as a soft material.	
Capability	High-speed simulation (in a few seconds) enables the simultaneous use of the simulator with experiment.	
Advantage to the conventional simulators	Overwhelmingly speedy compared with the conventional simulators. It can remove artifacts in an AFM image due to e.g. the defect of the probe tip.	
Application field	Inorganic/organic materials, nano-materials, organic soft materials, chemistry, pharmacy, bioscience	

FemAFM	Finite Element Method AFM Simulator	Classical theory
Property	It carries out the AFM simulation while taking into account the elastic deformation of the tip and the sample. It is suitable for micron-size sample. It performs the AFM image simulation for bio-materials such as proteins, DNA etc.	
Computing method and target	Assuming that the tip and the sample material obey the differential equation of elasticity, FemAFM solves it with the finite element method. It is suitable to simulate the AFM image and the frequency shift AFM image for a soft material.	
Capability	It equips the analysis tool based on the viscoelastic dynamics, and assumes to simulate polymers and a bio-materials. The frequency shift AFM image can be calculated by modeling the tip and the sample as the continuous elastic bodies.	
Advantage to the conventional simulators	In consideration of the users majoring in polymers and bio-materials, it treats the relatively macroscopic system.	
Application field	Inorganic/organic materials, nano-materials, organic soft materials, chemistry, pharmacy, bioscience	

LiqAFM	Soft Material Liquid AFM Simulator	Classical theory
Property	It faithfully simulates the cantilever motion in liquid. It is suitable for micron-size sample. It corresponds also to a viscoelastic sample.	
Computing method and target	It simulates the AFM in liquid. It is suitable to examine the resonance frequency of the cantilever in liquid, and the influence of the viscosity to the cantilever in liquid. It also simulates the force curve in case of a viscoelastic sample.	
Capability	It simulates the AFM in liquid with a cantilever having complex shapes. It equips the analysis tool based on the viscoelastic dynamics.	
Advantage to the conventional simulators	In consideration of the users majoring in bio-materials, it examines the viscoelastic behavior in liquid.	
Application field	organic materials, soft materials, chemistry, pharmacy, bioscience	

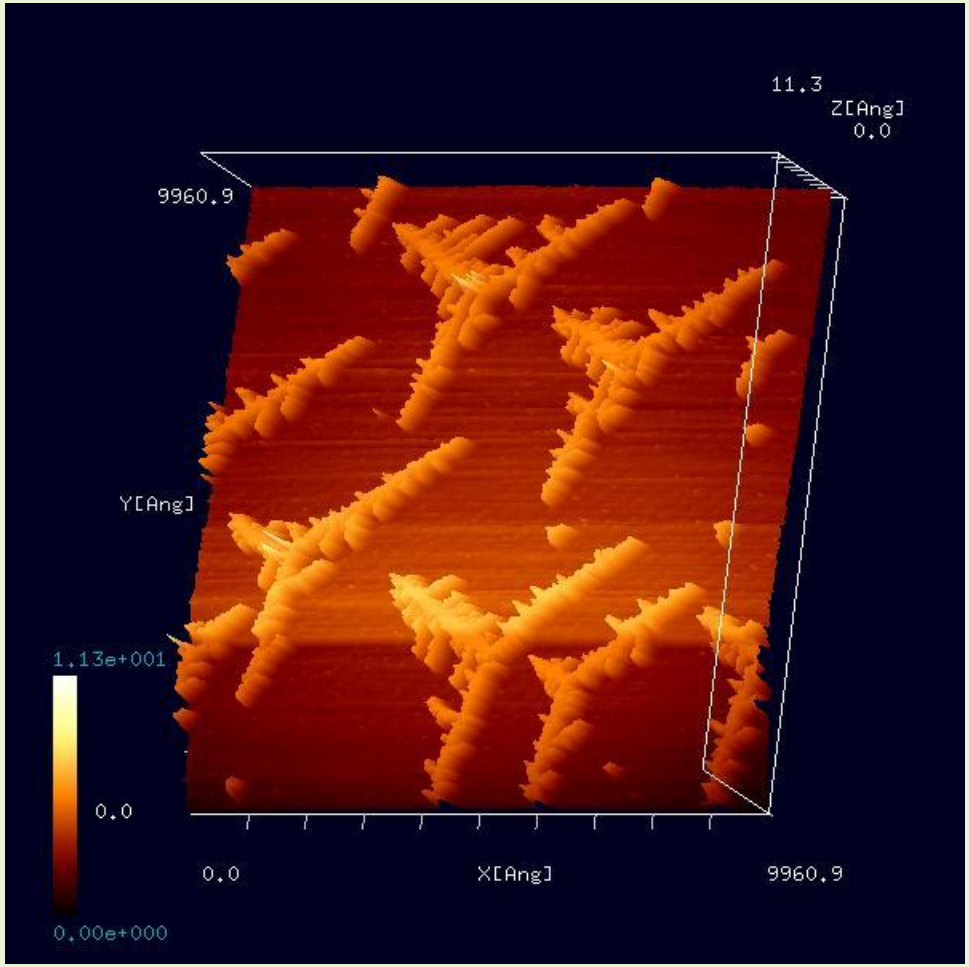
CG	Geometry Optimizing AFM Simulator	Classical theory
Property	It simulates the AFM image with the energy optimization of a molecular structure. It is suitable for molecular size. It can perform the frequency shift AFM image of a biopolymer.	
Computing method and target	It finds the stable conformation of a molecule by searching the energy minimum of the molecular system. It is suitable to examine relatively large scaled samples e.g. in case of calculation of the frequency shift AFM image of a polymer.	
Capability	It equips the frequency shift AFM image simulation.	
Advantage to the conventional simulators	It predicts the structure deformation of a sample molecule due to the interaction from the tip, taking into account the classical force parameter.	
Application field	Inorganic/organic molecular materials, biopolymers, proteins	

MD	Molecular Dynamics AFM Simulator	Classical theory
Property	It simulates the AFM image with the use of the molecular dynamics. It is suitable for molecular size. It performs the AFM force curve of a biopolymer.	
Computing method and target	It simulates the time evolution of a molecular system, where all the atoms are treated as the many-body system and the simultaneous Newton's equation of motion is solved. It is suitable to simulate the force curve when the tip is pushed into the sample molecule.	
Capability	It can evaluate the physical properties such as the force curve between the tip and the sample.	
Advantage to the conventional simulators	It is the most light-weighted simulator that treats the atomic/molecular many-body system with the molecular dynamics. It is therefore friendly to experimentalists.	
Application field	Inorganic/organic molecular materials, biopolymers, proteins	

DFTB	Quantum Mechanical SPM Simulator	Quantum theory
Property	It simulates AFM, STM, STS and KPFM of a sample surface. It is suitable for nano-size sample.	
Computing method and target	It simulates a frequency shift image, a tunneling current image, a local contact potential difference image, and a tunneling current spectrum. It adopts the tight binding calculation method based on the density functional theory, so that the simulation reduces a large calculation cost. It is suitable for nano-size sample such as a thin film of a semiconductor crystal.	
Capability	It performs STM simulation by the DFTB method with ease, equipped with seven kinds of element such as Si, W, Pt, Au, Ti, Al and Ru. It is the simplest simulator with the density functional theory among the marketplace.	
Advantage to the conventional simulators	It can obtain the equivalent results more quickly than the ones by conventional first-principle simulators. It may be the quantum theory simulator for experimentalists.	
Application field	Inorganic/organic materials	

SetModel	Atomic Structure Modeling Tool	
Property	It makes an atomic structure of a thin film of a crystal as you like, with easy operations.	
Capability	It makes any thin film of a crystal that the users would like to prepare. The users construct their own atomic model available for solvers in the SPM Simulator by themselves. The resulted model data are available to the five solvers (GeoAFM, FemAFM, CG, MD, DFTB) as a tip or a sample model. Everyone can start up the tool with ease due to the satisfactory graphical user interface.	
Advantage to the conventional simulators	It drastically reduces difficult tasks to make an initial model data for the simulation. Users do not need technical knowledges.	
Application field	Inorganic crystal structure, organic/inorganic semiconductor	

Analyzer	Digital image processor	
Property	It performs the digital processing of the SPM experimental data and the simulated image data together.	
Application field	Inorganic/organic materials, nano-materials, organic soft materials, chemistry, pharmacy, bioscience	



It can load the experimental binary data from SPM devices produced by leading companies in the marketplace; such as Asylum Research, Omicron Nanotechnology, UNISOKU, Digital Surf etc.

It makes the original experimental SPM images more impressive, by various functions; the 3D view, the tilt adjustment etc.

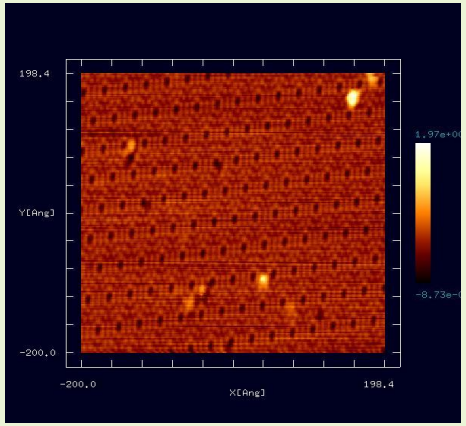
The image is provided by Fukutani laboratory in the Institute of Industrial Science, the University of Tokyo.
The Au islands grown on Ir surface. The deposition and the annealing makes the self-forming fractal islands.
S. Ogura *et al*., Phys. Rev. B **73**, 125442 (2006); S. Ogura and K. Fukutani, J. Phys.: Condens. Matter **21** (2009) 474210.]

Blind Reconstruction method (Estimation of tip shape)

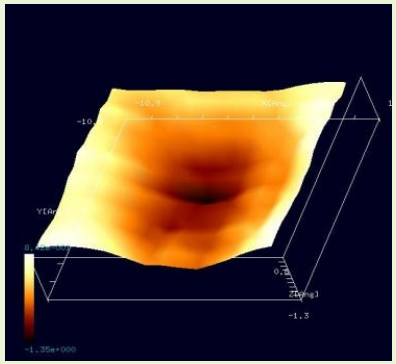
- Since the tip shape estimation is a kind of inverse problem, there are infinite candidates of the estimated tip shape from one experimental image.
- Users can select a desirable tip shape.
- The radius of curvature at the top of the tip can be evaluated.

- Users can select an optimized tip shape that reproduces the standard sample shape well.
- Users are able to estimate a tip shape suitable for their purpose.

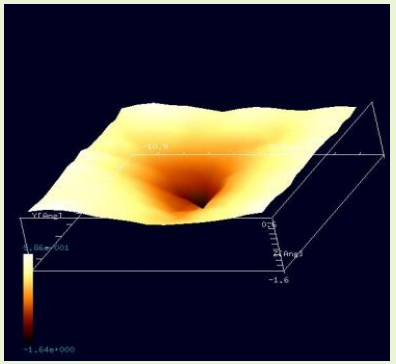
It shows a great power to calibrate an artificial structure, e.g. the semiconductor nano-devise



Which is the optimum solution among infinite candidates of the estimated tip shape?



or



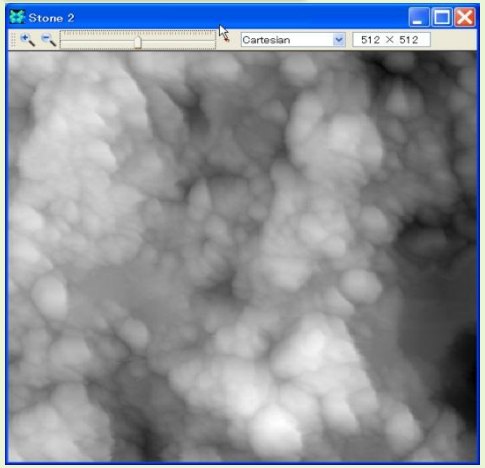
It is superior to the tip shape estimation function attached to SPIP, Gwyddion

Image processing by Fourier analyses

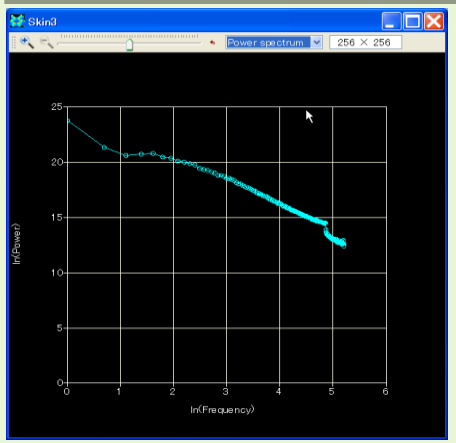
Application field Soft materials, bio-materials

It removes some spectrum components, so that the kinks or the wrinkles of a sample surface are corrected. It takes a great effect when treating soft sample materials such as a living thin film.

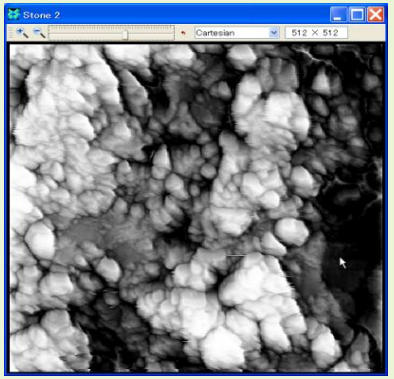
Original image

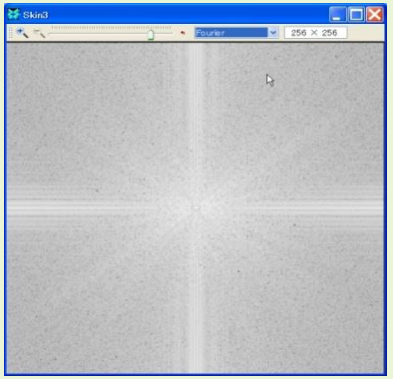


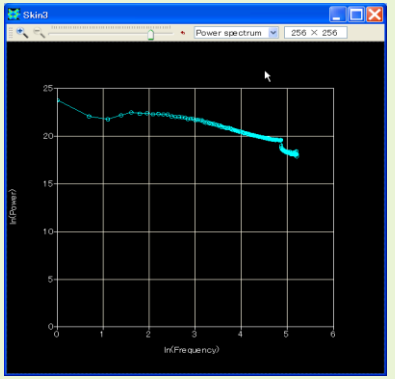
Original power spectrum



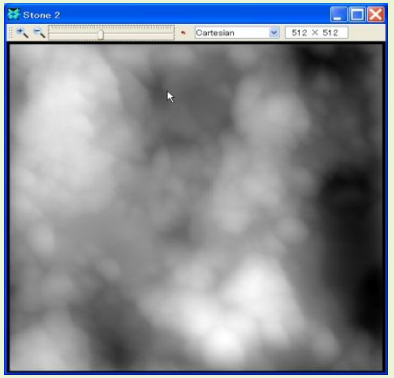
Emphasize high frequencies

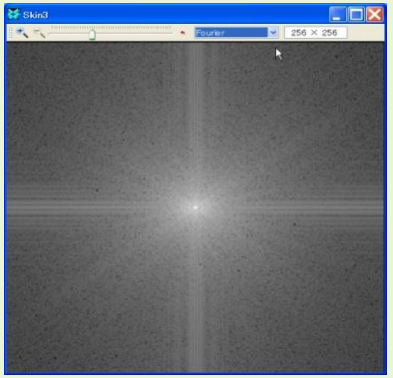


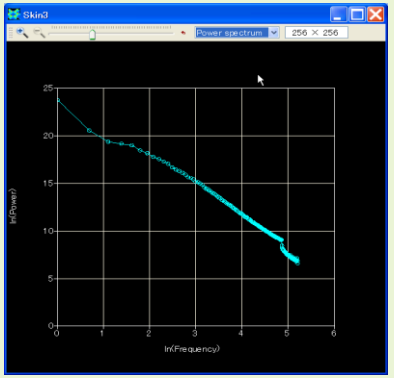




Emphasize low frequencies



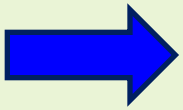




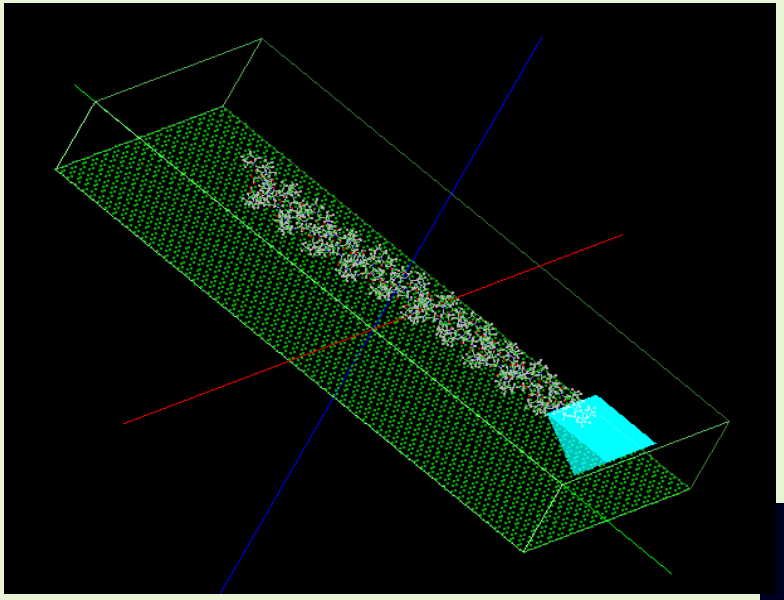
Cartesian | Fourier | Power Spectrum

FemAFM	Finite Element Method AFM Simulator	Classical theory
Property	It carries out the AFM simulation while taking into account the elastic deformation of the tip and the sample. It equips the analysis tool based on the viscoelastic dynamics, and assumes to simulate polymers and a bio-materials. It performs the AFM image simulation for bio-materials such as proteins, DNA etc.	
Application field	Inorganic/organic materials, nano-materials, organic soft materials, chemistry, pharmacy, bioscience	

- Assuming that each of the tip and the sample material is the continuous elastic body made of single compound, FemAFM solves the differential equation of elasticity with the finite element method.
- The van der Waals interaction between a tip and a sample material is taken into account.
- It assumes in a vacuum environment or in the air at room temperature. (The simulation in liquid can be performed by the LiqAFM.)
- Absolutely classical theory. (The quantum mechanical approach can be performed by the DFTB.)



It is well suited for the AFM simulation in macroscopic scale.



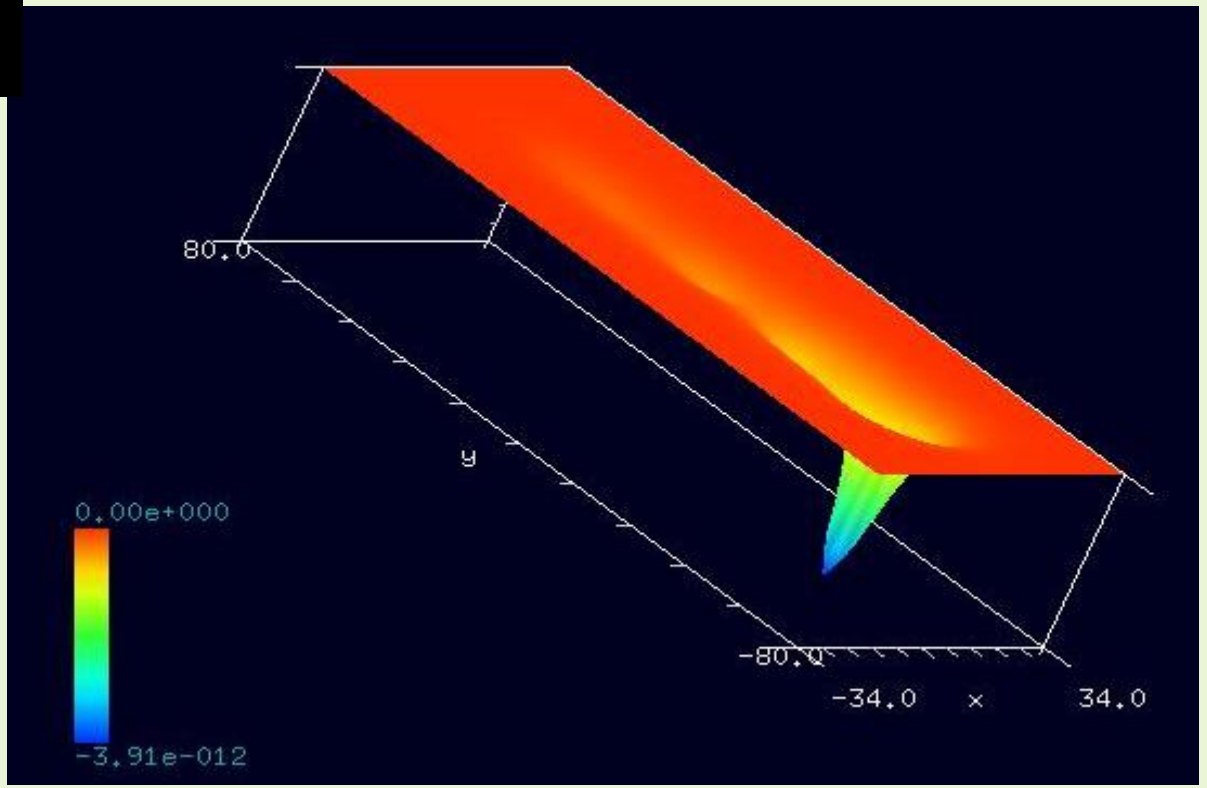
Useful tool for the AFM analyses of polymers

Sample:

a single molecule of Glycoprotein (1clg) on HOPG（Highly Oriented Pyrolytic Graphite）

Tip:

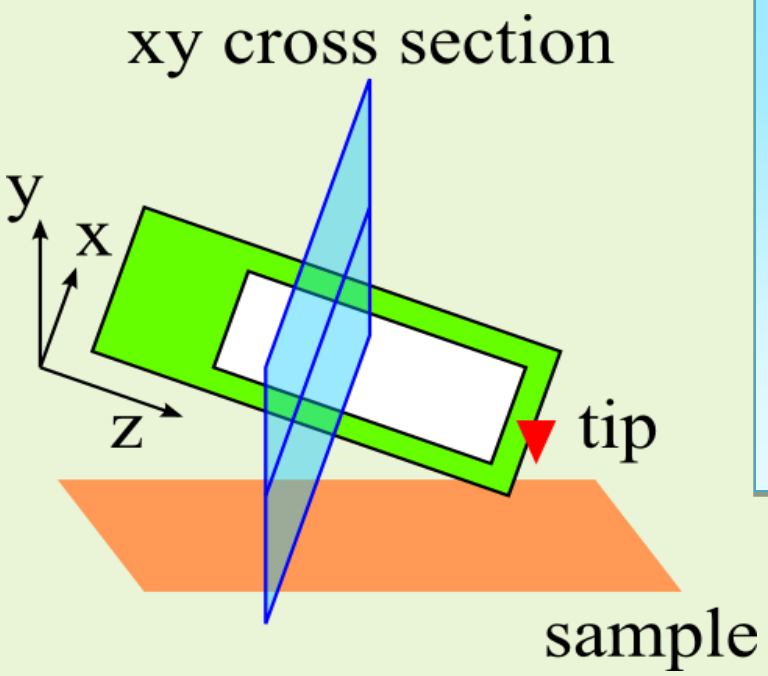
pyramidical



Simulated AFM image:

Due to the van der Waals force, the attractive force to the top of the tip rapidly increases even as the tip comes close a little.

LiqAFM	Soft Material Liquid AFM Simulator	Classical theory
Property	It faithfully simulates the cantilever motion in liquid for micron-size sample.	
Application field	organic materials, soft materials, chemistry, pharmacy, bioscience	

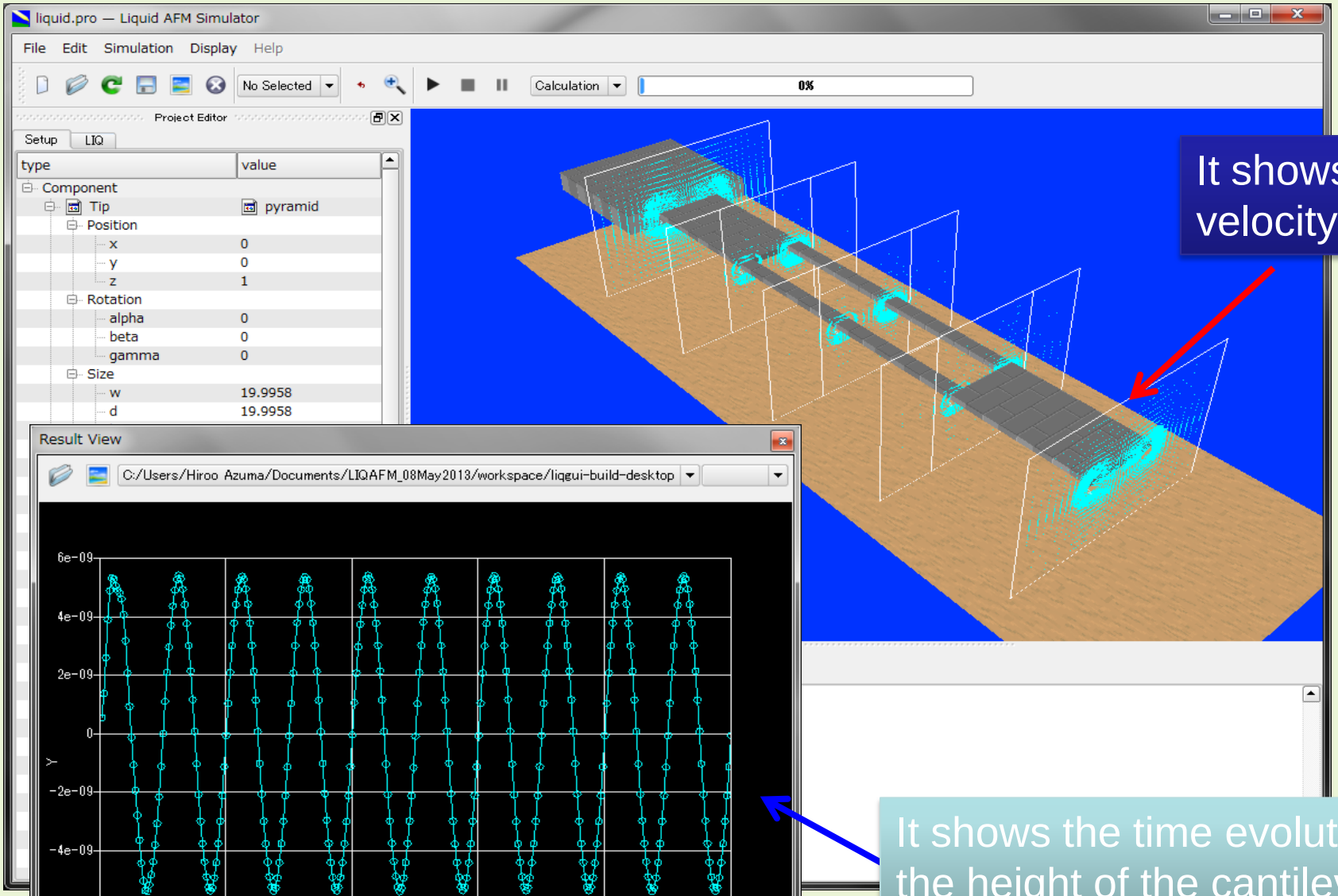


- It simulates a cantilever motion in liquid.
- The cantilever motion is treated as the one-dimensional problem along z-direction.
- The fluid flow is treated as the two-dimensional problem in xy-cross section.
- It considers the viscosity of the fluid and the elasticity of the sample.

It is well suited for the AFM simulation of living materials in liquid in macroscopic scale.

LiqAFM Overview

It easily acheives the resonance frequency analysis of the cantilever

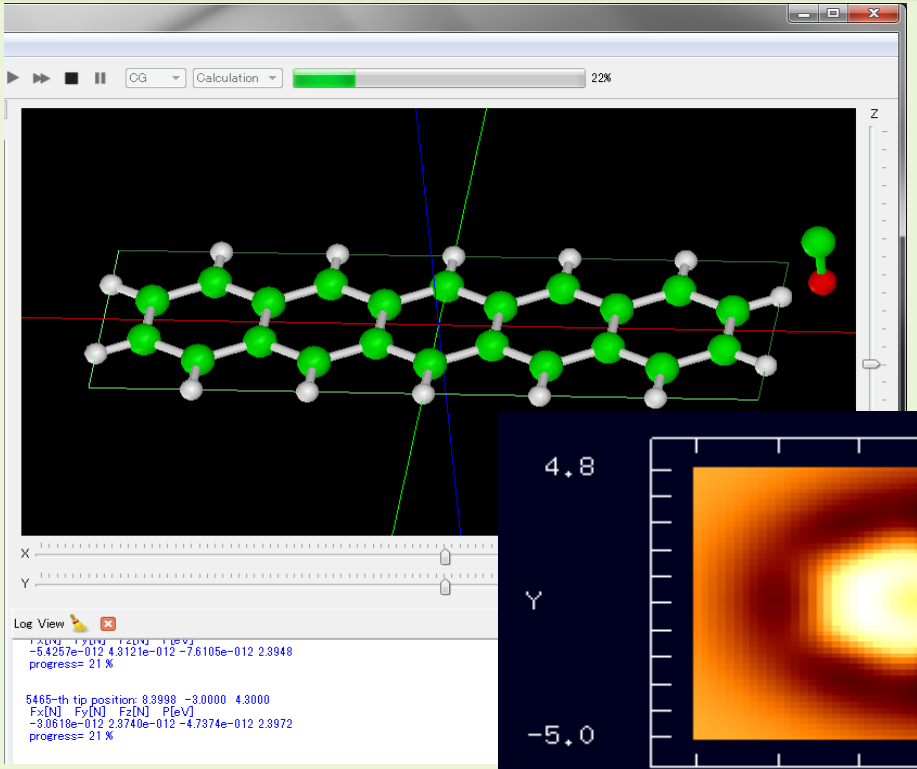


It shows the fluid velocity vectors

It shows the time evolution of the height of the cantilever.

CG	Geometry Optimizing AFM Simulator	Classical theory
Property	It finds the stable conformation of a molecule by searching the energy minimum of the molecular system. It is suitable to examine e.g. organic molecule samples in the classical theory.	
Application field	Inorganic/organic materials, biopolymers, proteins	

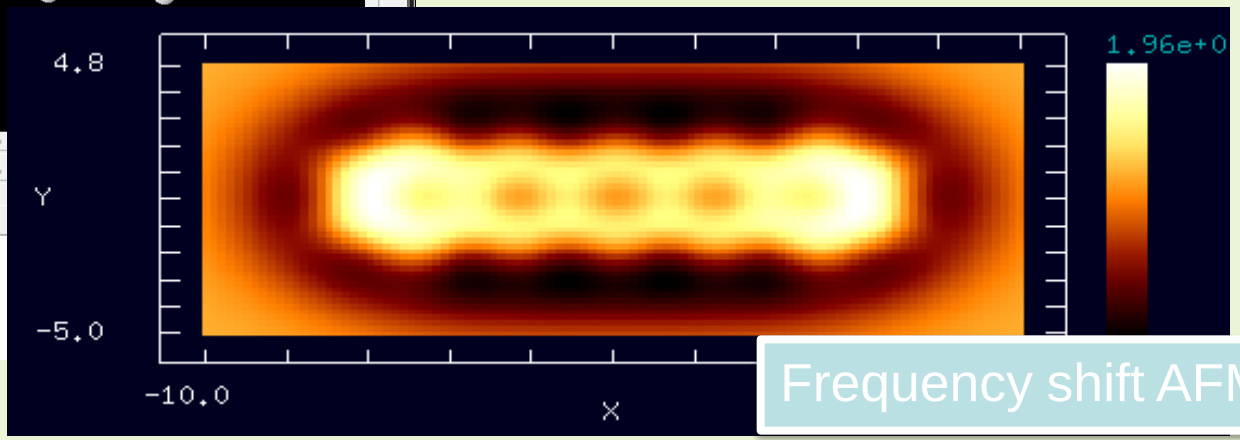
AFM image simulation of a pentacene molecule using a CO molecule tip.



Deviation from a resonant frequency

$$\Delta f = r f_0 = -\frac{f_0}{2kA\pi}\int_0^{2\pi} F(A\cos\theta + L)\cos\theta \,\mathrm{d}\theta$$

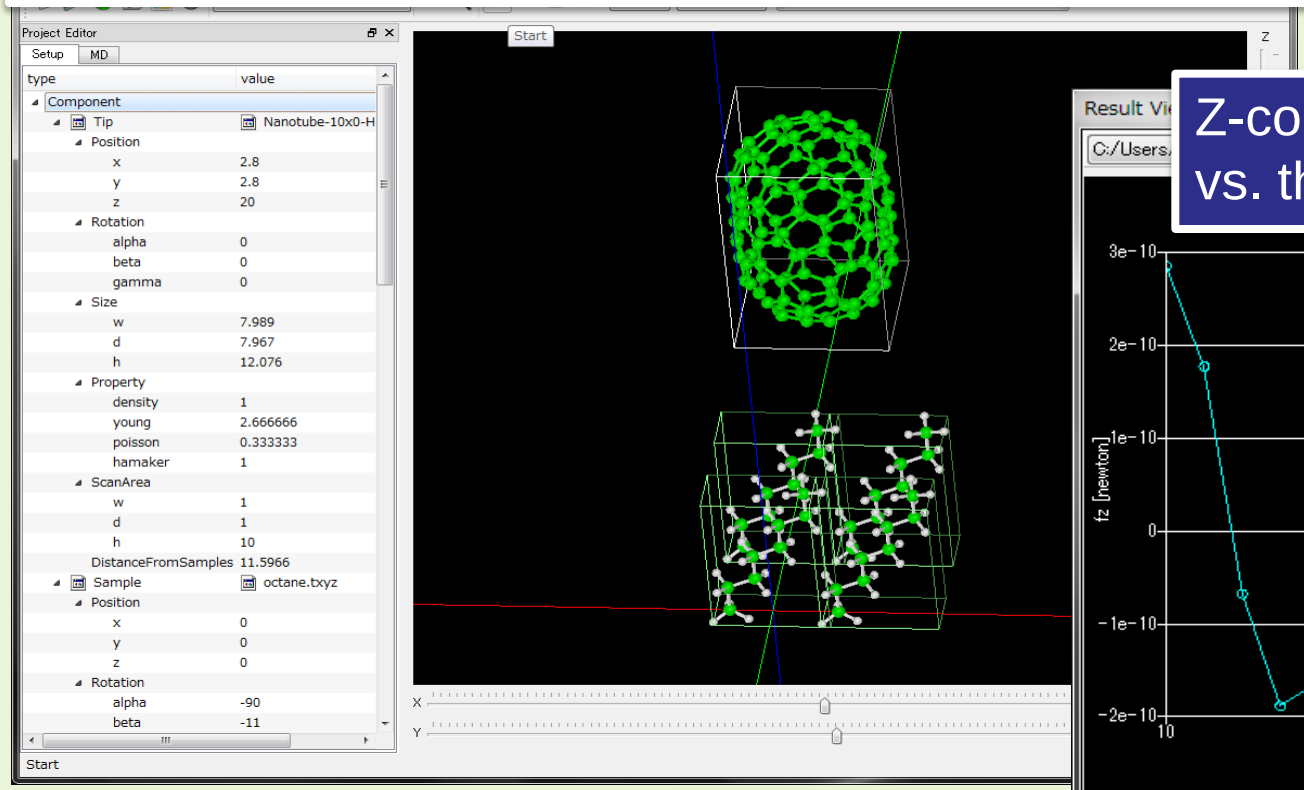
Interaction force between the tip and the sample



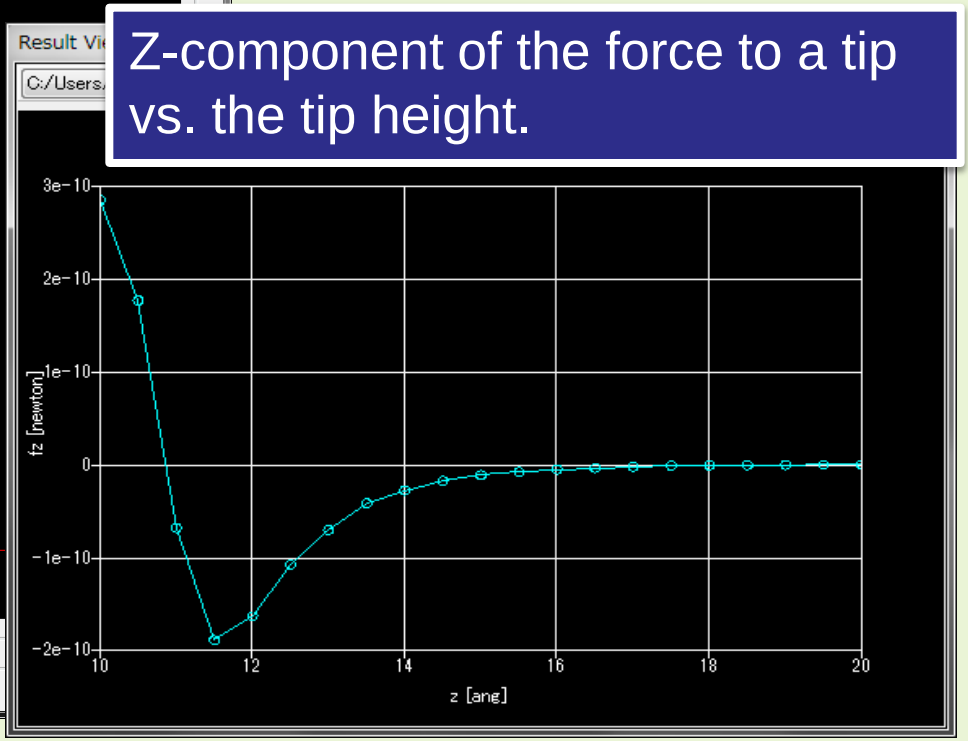
Frequency shift AFM image

MD	Molecular Dynamics AFM Simulator	Classical theory
Property	It simulates the time evolution of a molecular system, where all the atoms are treated as the many-body system and the simultaneous Newton's equation of motion is solved. It is suitable to simulate the deformation of an organic molecule samples in classical theory.	
Application field	Inorganic/organic materials, biopolymers, proteins	

Force curve simulation of the four octane molecules using the carbon nanotube tip.



Z-component of the force to a tip vs. the tip height.

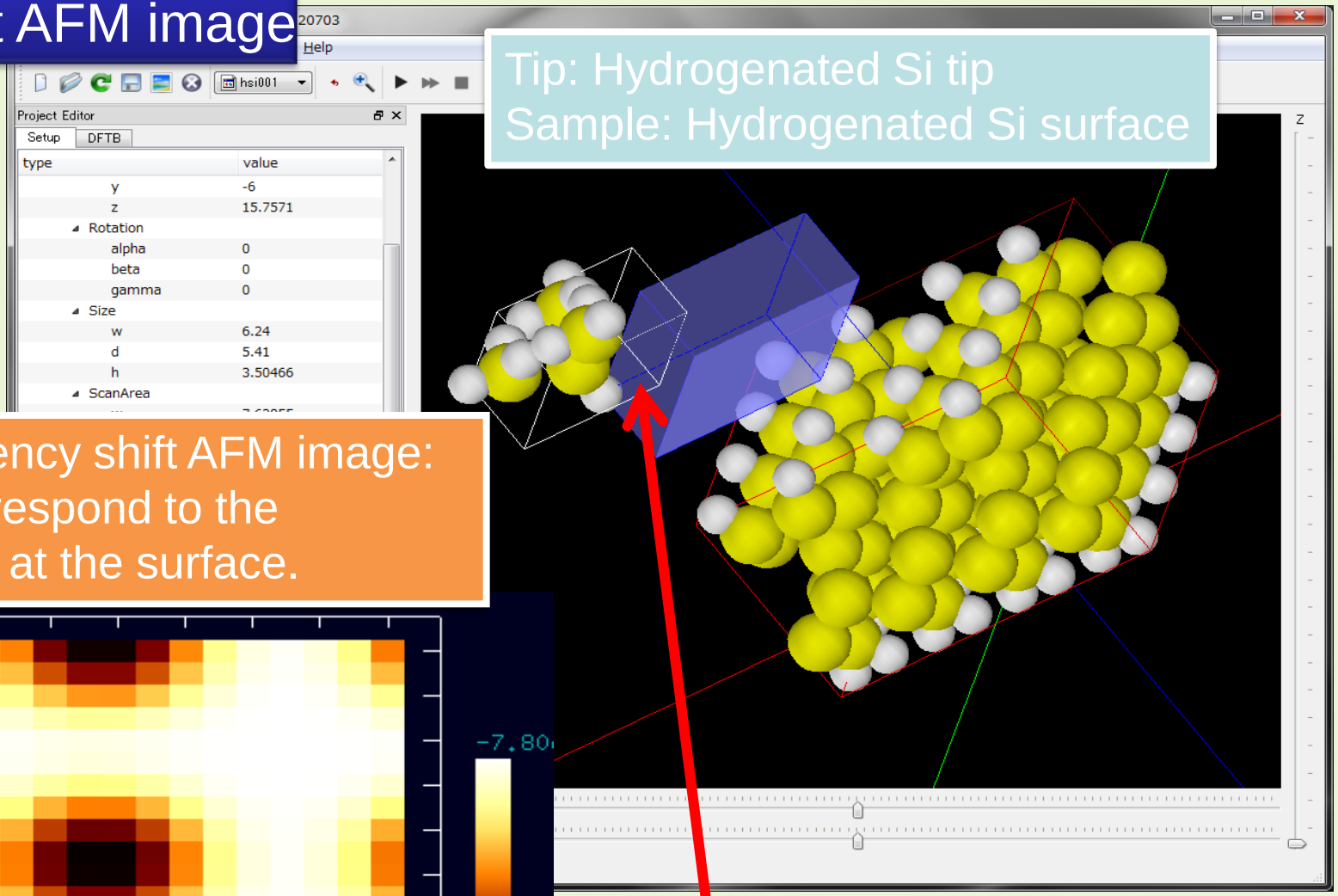


DFTB	Quantum Mechanical SPM Simulator	Quantum theory
Property	Simulates AFM, STM, STS and KPFM of a sample surface in atom-scale.	
Application field	Inorganic/organic materials	

- Adopts the tight binding calculation method based on the density functional theory.
  Deals with the quantum chemical problems based on the first principle calculation.
- Simulation targets:
  - Frequency shift AFM image
  - Tunneling current image (STM)
  - Tunneling current spectrum (STS, simulates the differential conductivity of the tunneling current is propotional to the local density of states.
  - KPFM (local contact potential difference image)
  - etc…

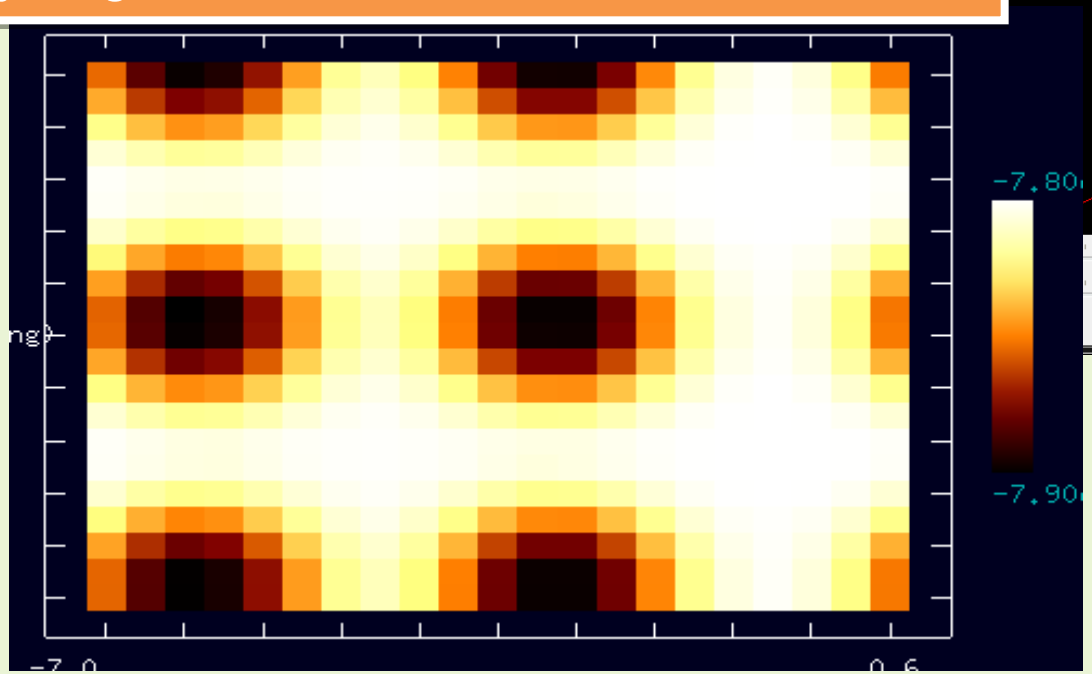
→ Simulates the STM image as precise as possible in microscopic atom-scale.

Frequency shift AFM image



Tip: Hydrogenated Si tip
Sample: Hydrogenated Si surface

Result of the Frequency shift AFM image:
The dark points correspond to the hydrogens attached at the surface.

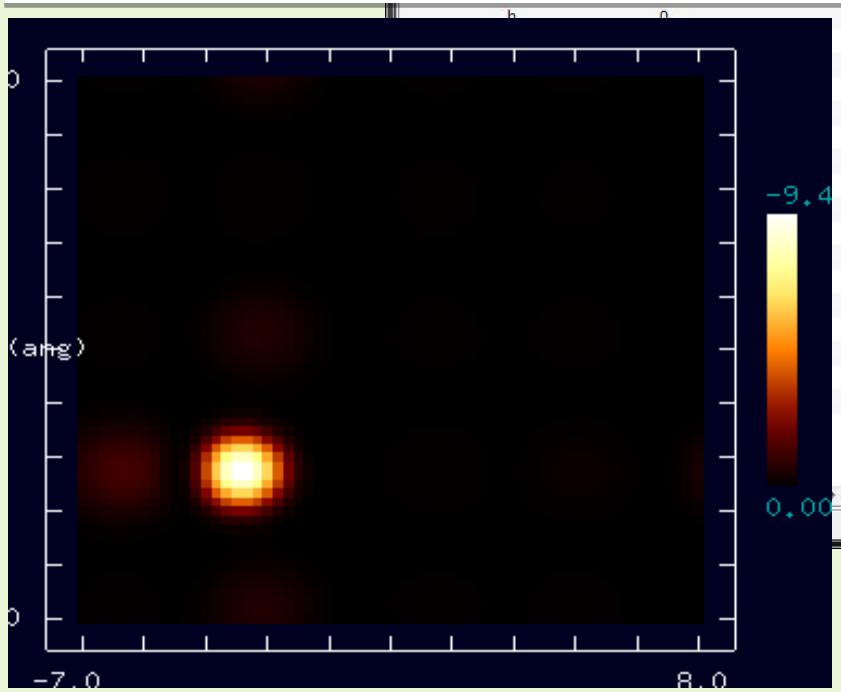


Scanning area

STM image (Tunneling current image)

Tip: Hydrogenated Si tip
Sample: Hydrogenated Si surface

Result of the STM image:
The large current shows that there is a dangling bond where a hydrogen atom is lacked.

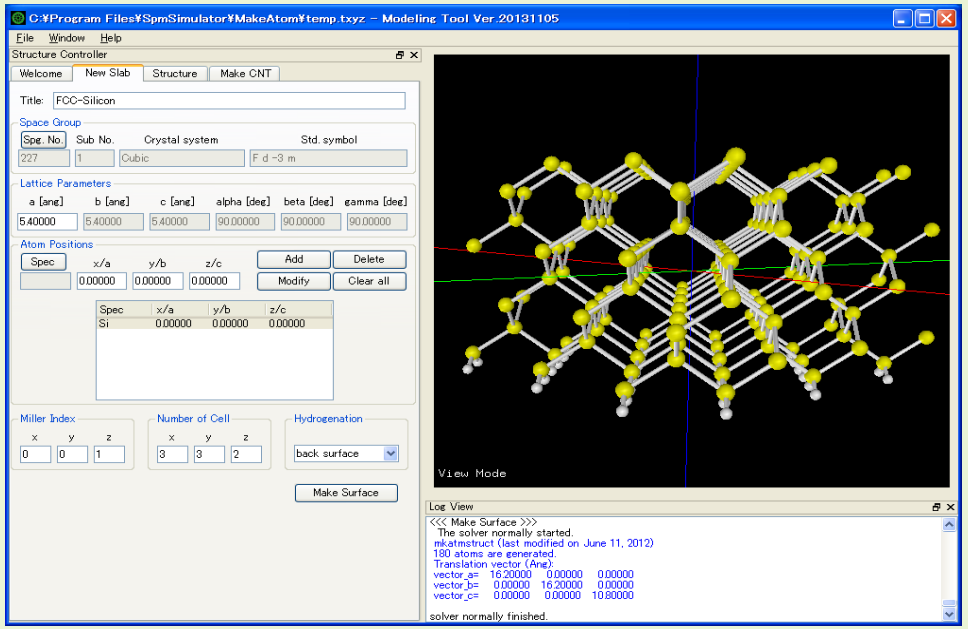


A hydrogen at one cite is lacked.

SetModel	Atomic Structure Modeling Tool	
Property	Makes an atomic structure of a thin film of a crystal as you like, with an easy operation.	

Creation of a thin film or a tip model

The modeling tool is bundled with the SPM Simulator.



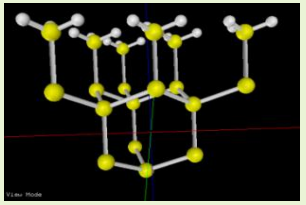
(1) Creates atomic models for the SPM Simulator. 3D-view lets you see in an intuitive manner.

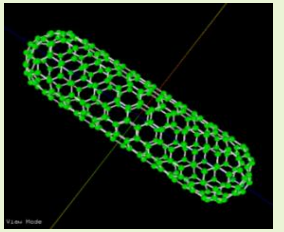
(2) Creates any thin film of a lattice easily by the lattice information.

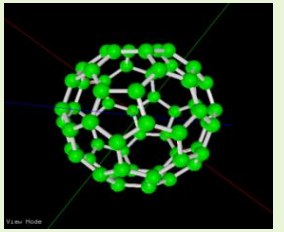
(3) Creates a tip model by cutting from the lattice.

(4) Replaces, moves, deletes, rotates, etc. any atoms in the model.

(5) Creates various shaped carbon nanotubes and fullerenes easily.



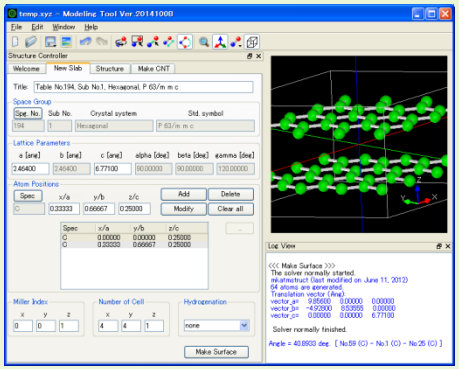


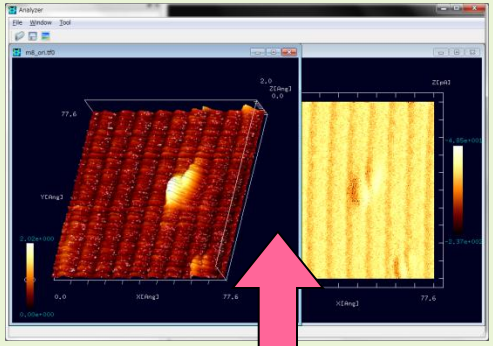


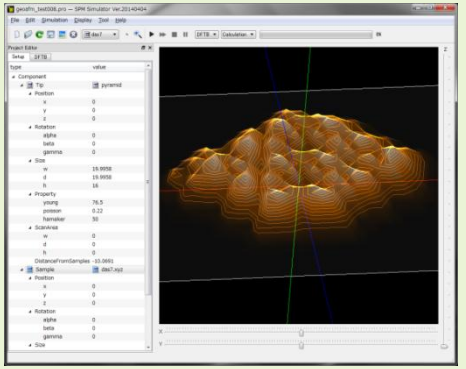
Creation of a molecular sample model

The freewares, ChemSketch and OpenBabel are available.

SPM Case Examples of Calculation



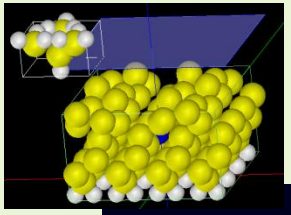


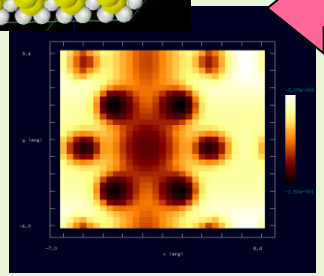


Analyzer
The Experimental Image Data Processor

SetModel
Atomic Structure Modeling Tool

GeoAFM
Geometrical Mutual AFM Simulator

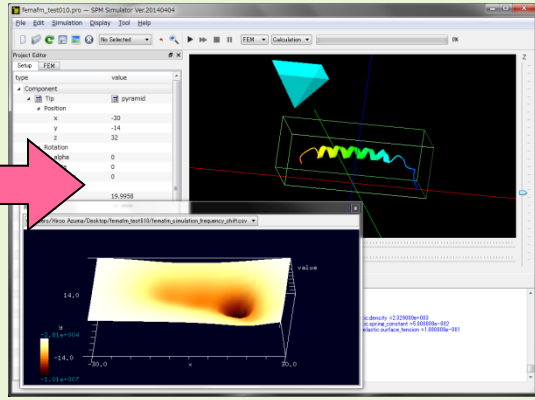




DFTB
Quantum Mechanical SPM Simulator

SPM Simulator

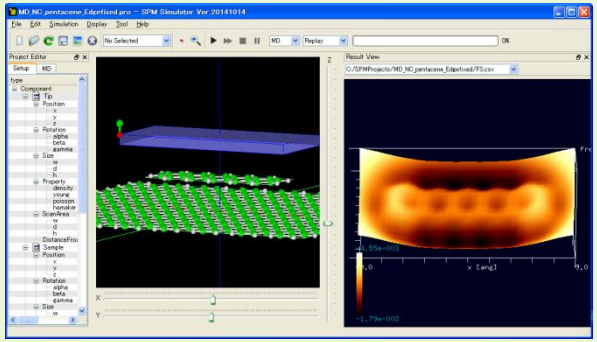
FemAFM
Finite element method AFM simulator

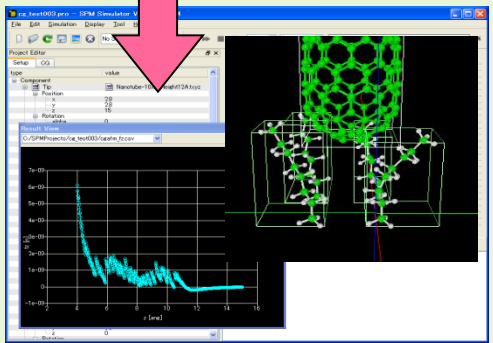


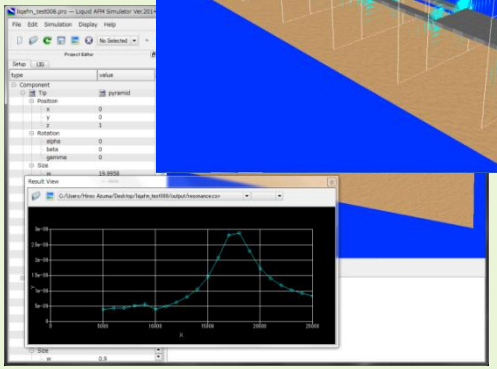
MD
Molecular Dynamics AFM Image Simulator

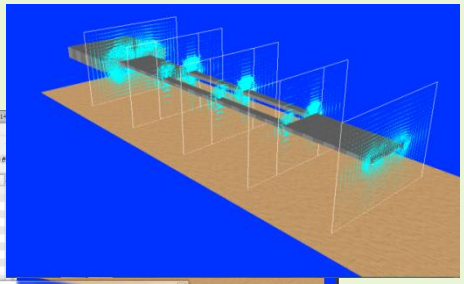
CG
Geometry Optimizing AFM Image Simulator

LiqAFM
Soft Material Liquid AFM Simulator





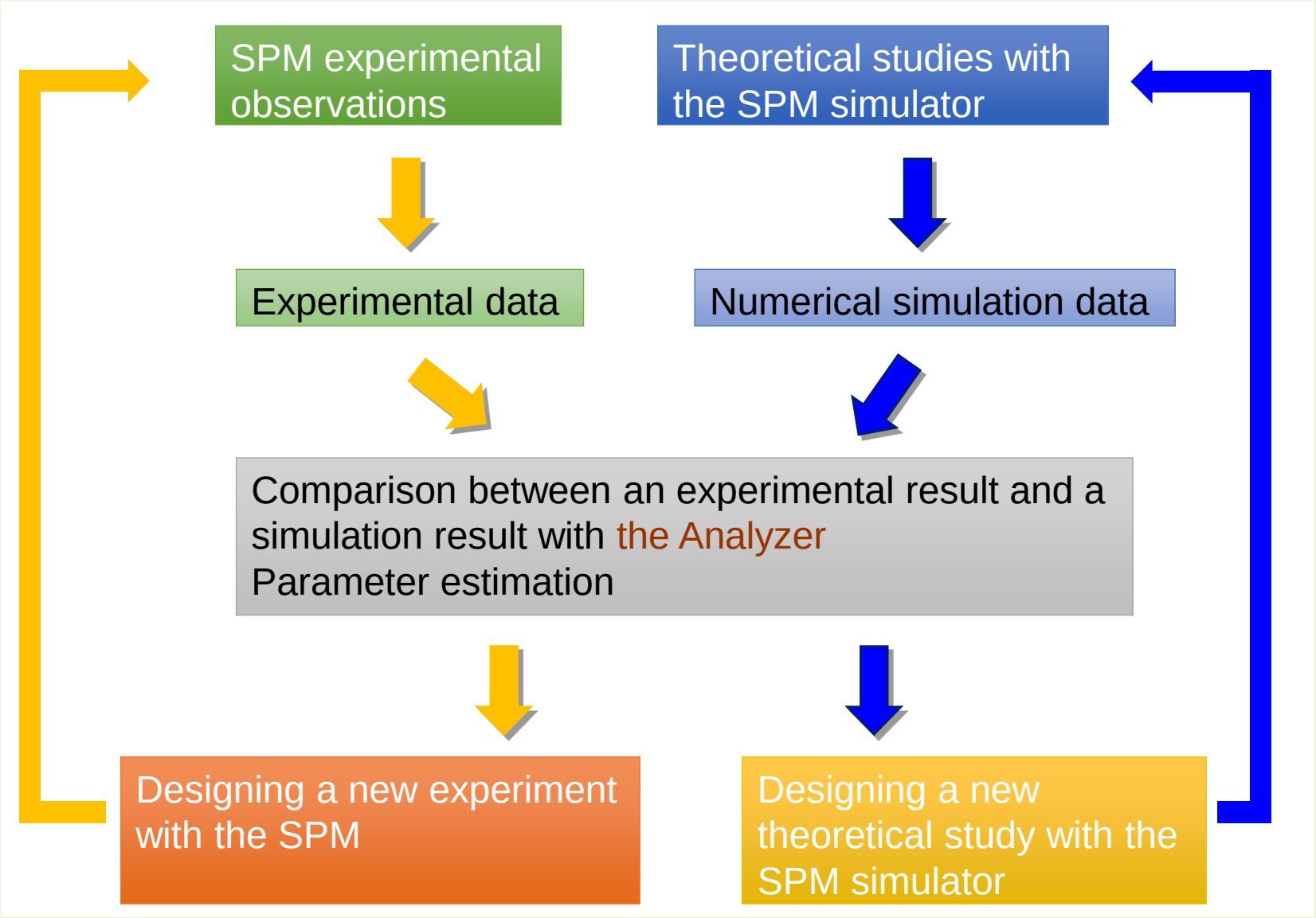




Comparison and Verification Function between the Experimental Image and the Simulated Image

Analyzer

It handles the SPM experimental data and the simulated image data uniformly.

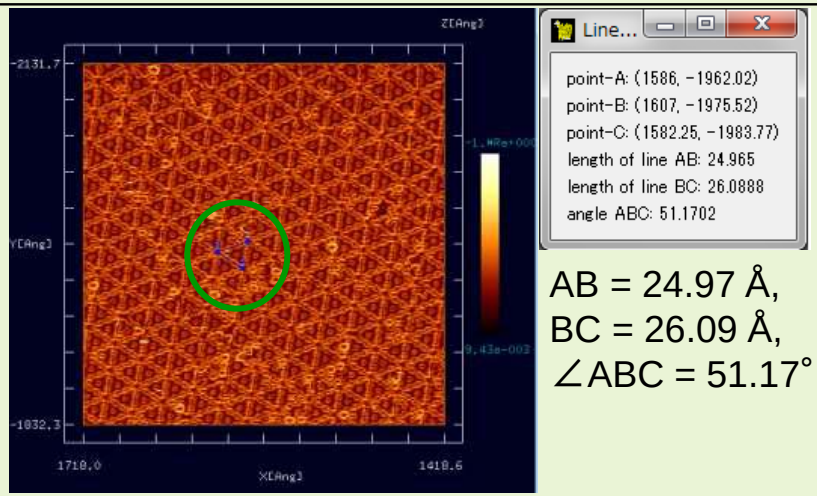


Example of the Comparison Between an AFM Experiment and a Simulation of Si(111)-(7x7) DAS

Analyzer

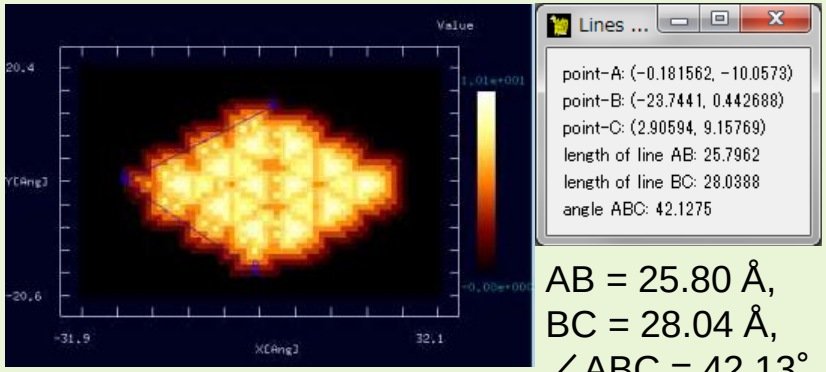
Comparison and measurement of the length and the angle of the lattice

Experimental image



AB = 24.97 Å,
BC = 26.09 Å,
∠ABC = 51.17°

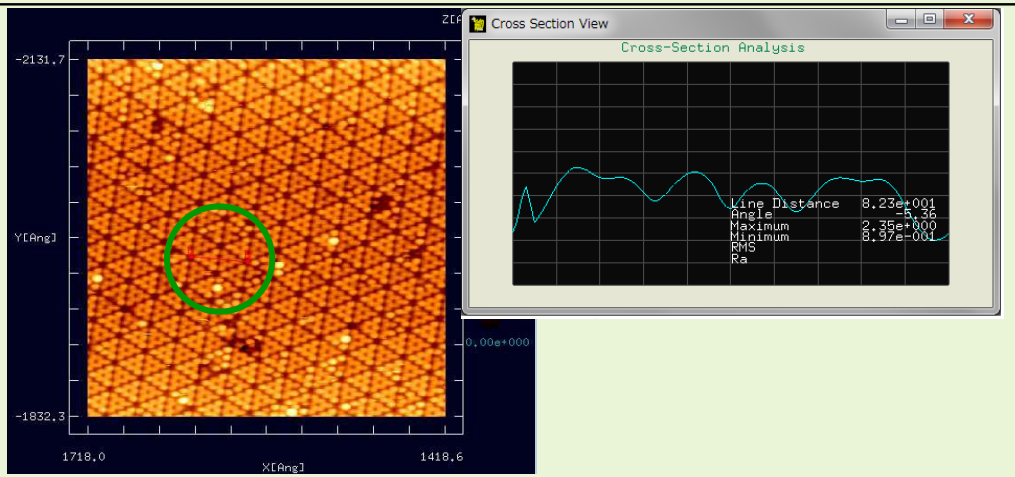
Simulation result obtained with the GeoAFM



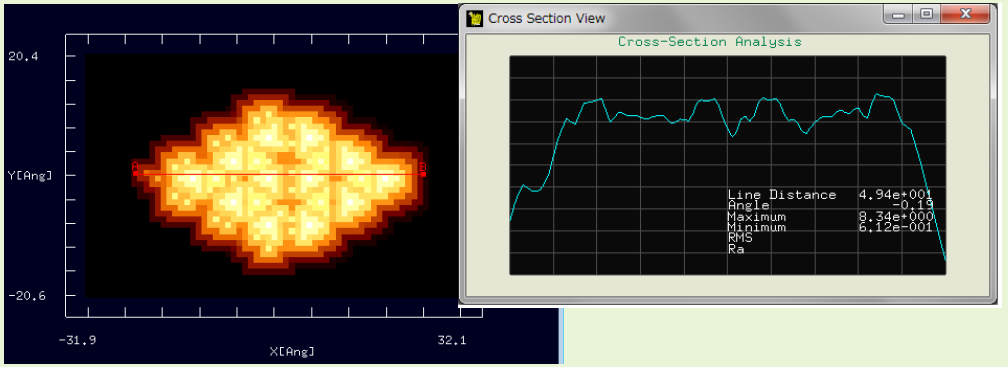
AB = 25.80 Å,
BC = 28.04 Å,
∠ABC = 42.13°

(loaded the simulation result obtained with the GeoAFM)

Comparison of the cross sections of the SPM images



(The original image is provided by Professor Hiroyuki Hirayama, Nano-Quantum Physics at Surfaces and Interfaces, Department of Materials and Engineering, Tokyo Institute of Technology.)



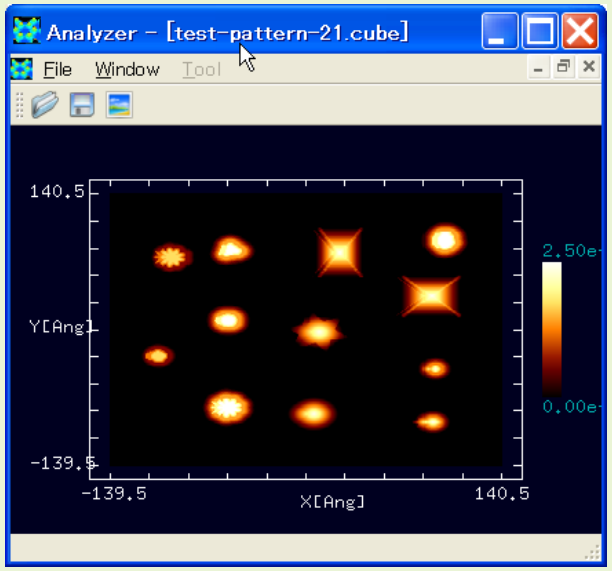
(loaded the simulation result obtained with the GeoAFM)

All these can be done on the same platform.
The comparison gives us a plan to simulate better.

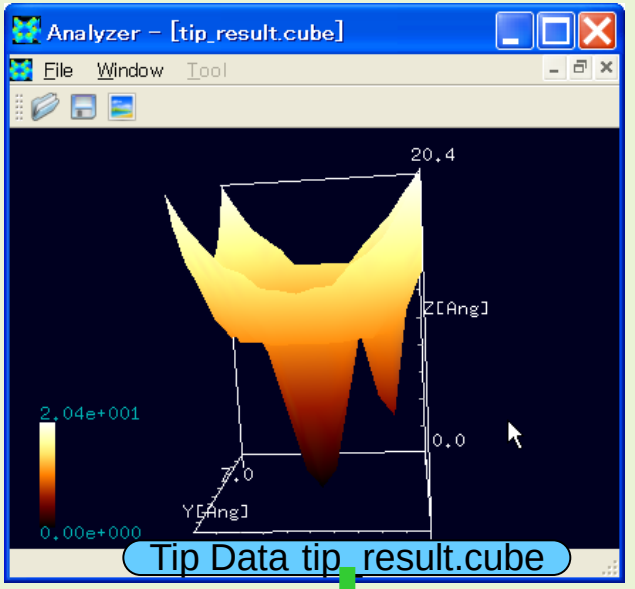
The Blind Tip Reconstruction Method & Removing the Artifacts from Experimental Images (1)

The blind tip reconstruction method

The blind tip reconstruction and removal of the artifacts, for an artificial AFM image by a broken double-tip.

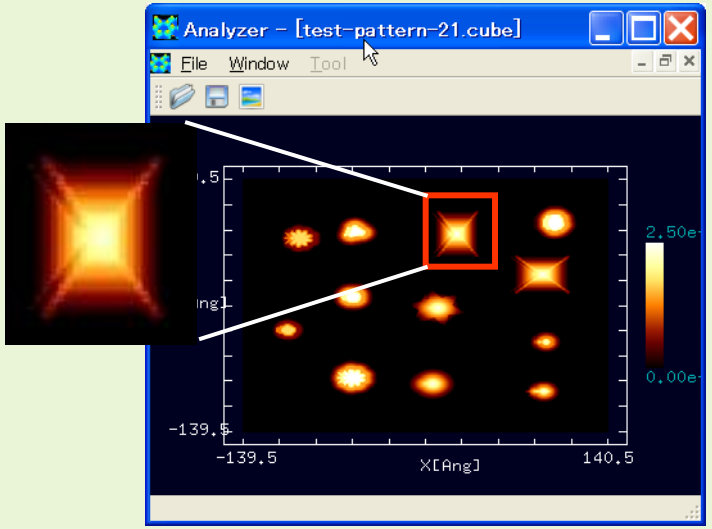


Estimation with the blind tip reconstruction method using the parameter you set (0.0~1.0)
0.0 : the maximum blind tip
1.0 : the minimum blind tip

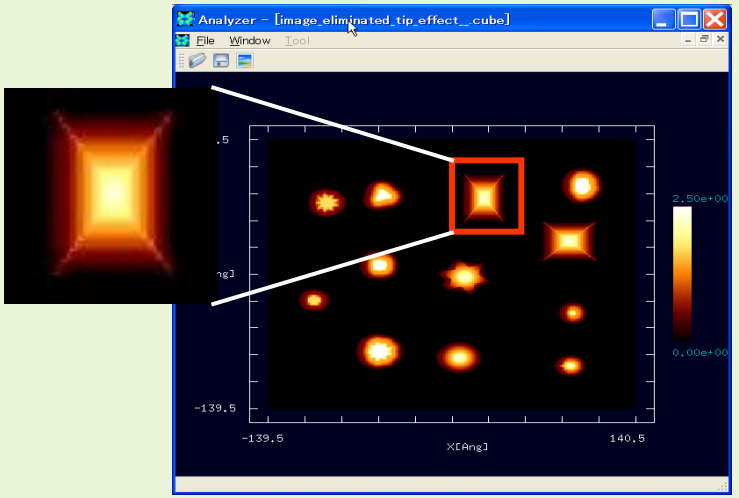


Tip Data tip_result.cube

Removing the artifacts from experimental images



Removing the artifacts with the specified tip data

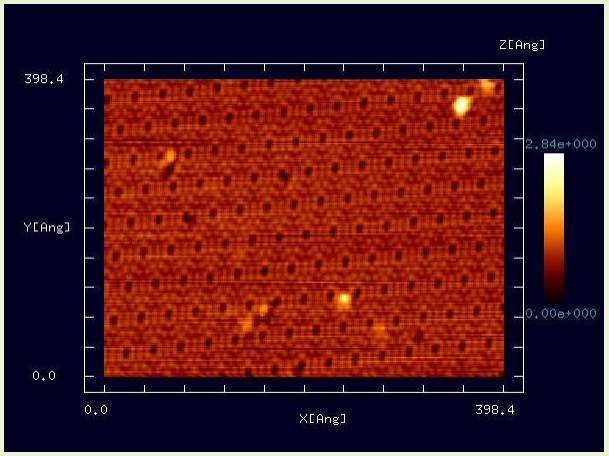


The Blind Tip Reconstruction Method & Removing the Artifacts from Experimental Images (2)

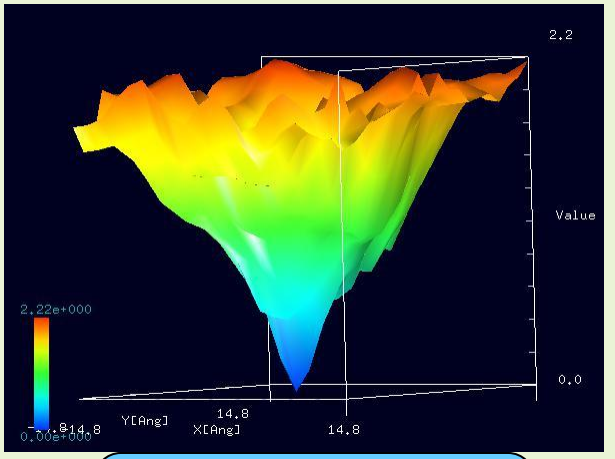
Analyzer

The blind tip reconstruction method

The blind tip reconstruction and removal of the artifacts, for an original SPM image by an unknown tip.

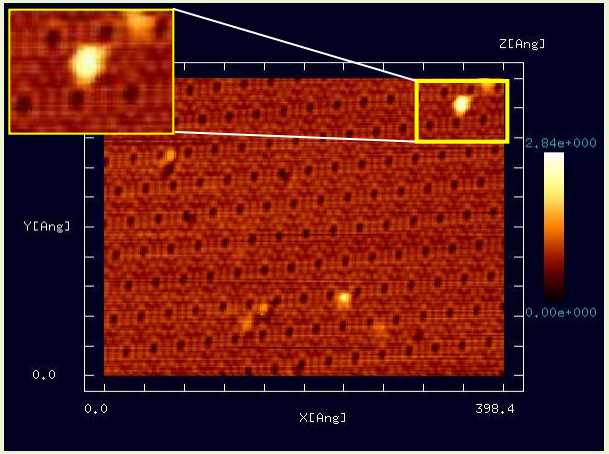


Estimation with the blind tip reconstruction method using the parameter you set (0.0~1.0)
0.0 : the maximum blind tip
1.0 : the minimum blind tip

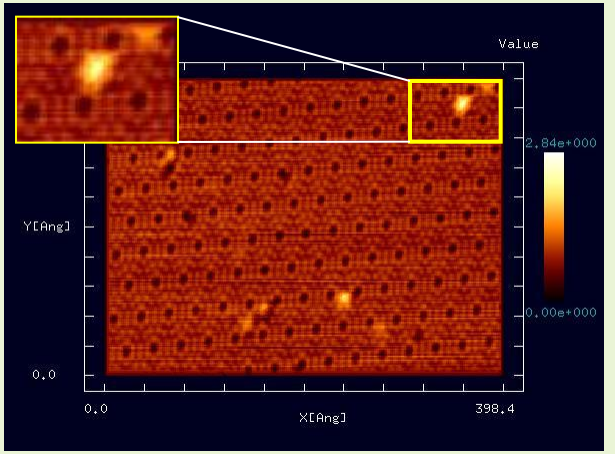


Tip Data tip_result.cube

Removing the artifacts from experimental images



Removing the artifacts with the specified tip data

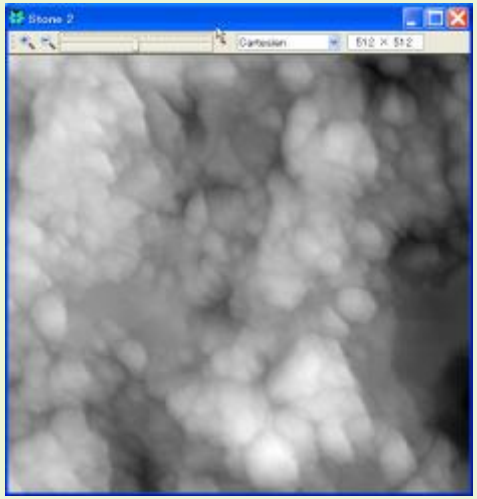


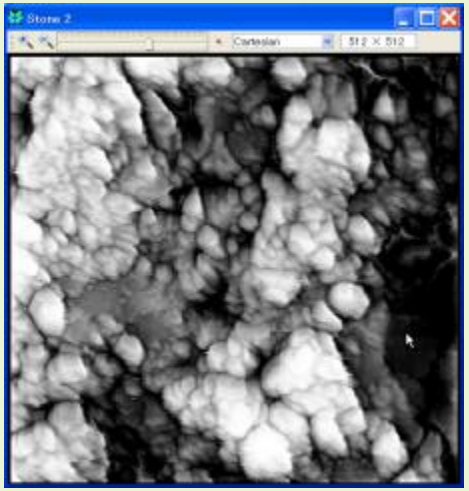
(The original image is provided by Professor Katsuyuki Fukutani, Vacuum and Surface Physics, Institute of Industrial Science, The University of Tokyo.)

Fourier Analysis of the Image

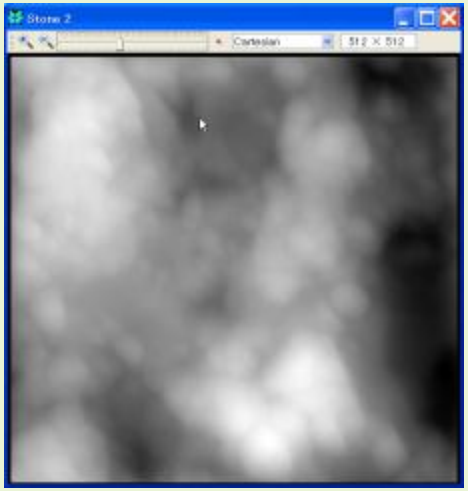
Analyzer

Fourier analysis of the image

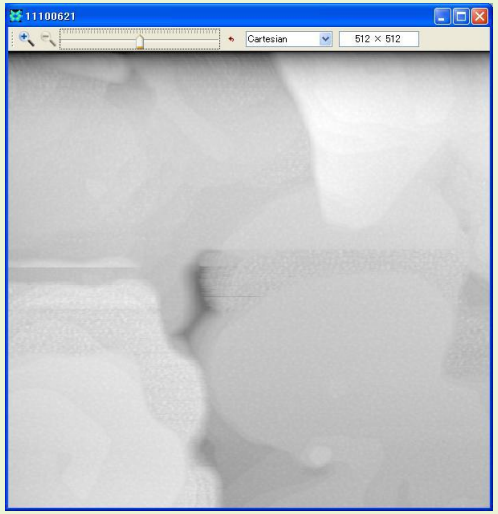


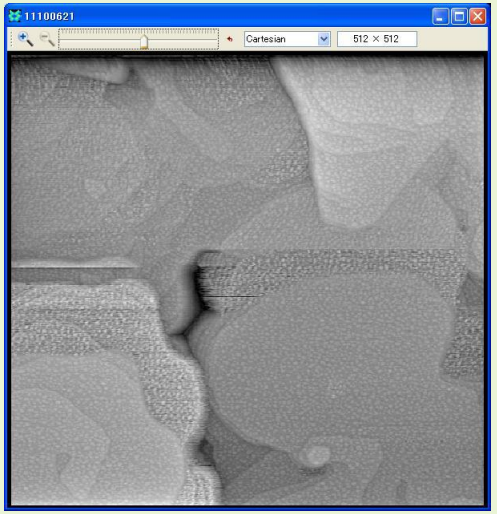


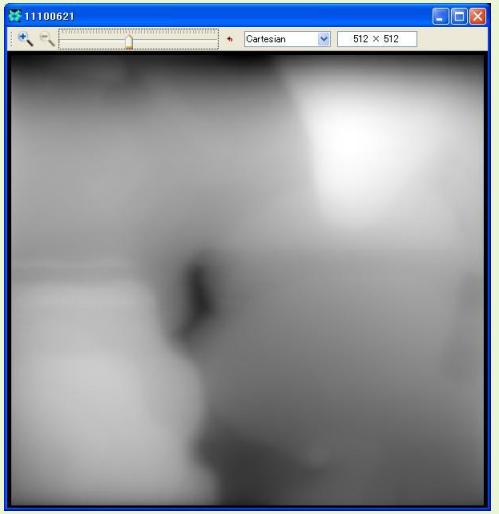
Emphasize high frequencies



Emphasize low frequencies



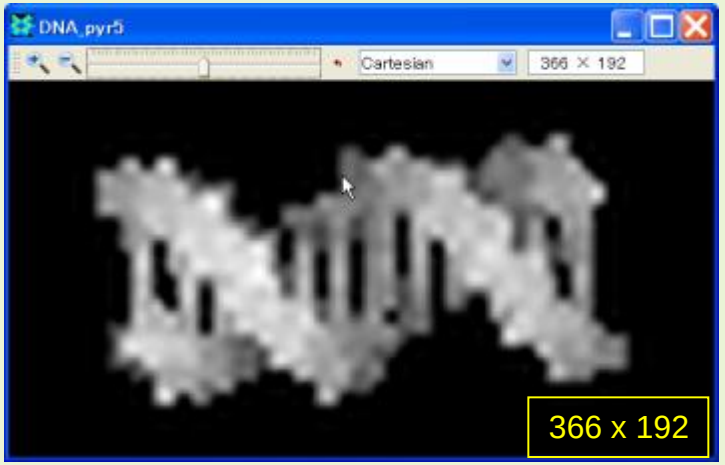


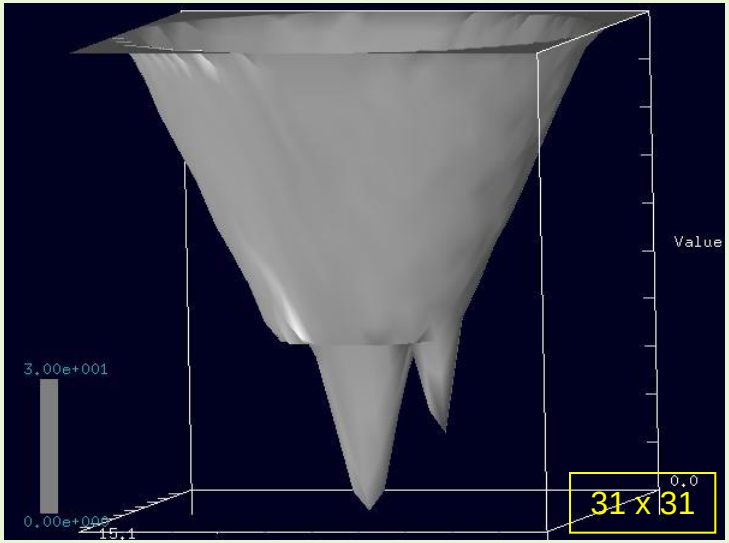


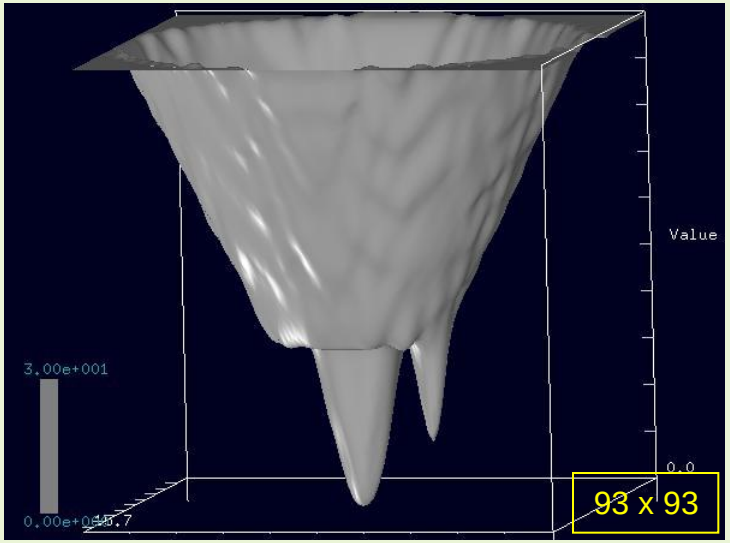
Improvement of the Subjective Quality of the Image

Analyzer

Improvement of the subjective quality of the image

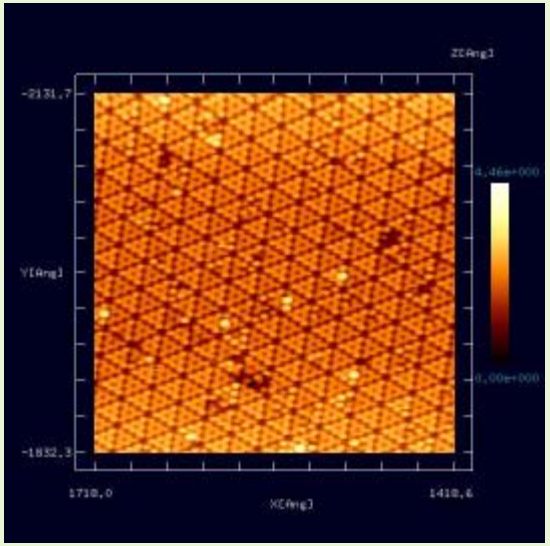




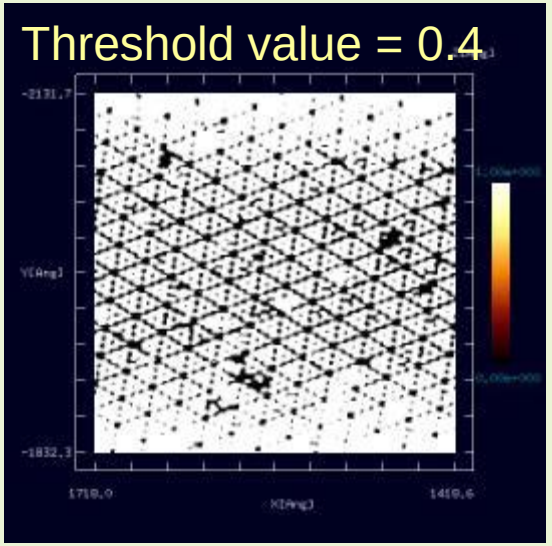


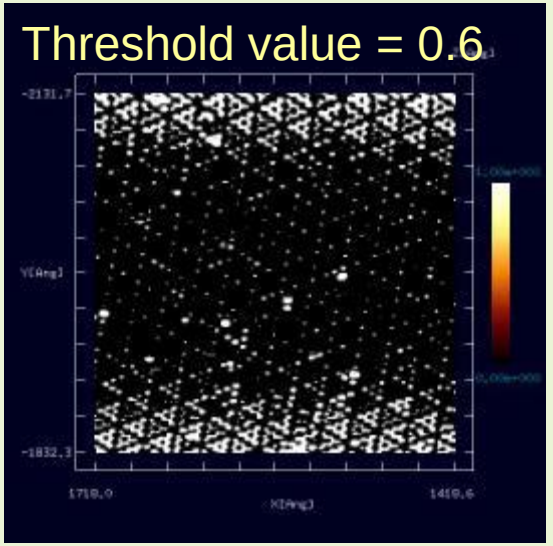
Digital Image Processings Function (1)

Thresholding for creating binary images



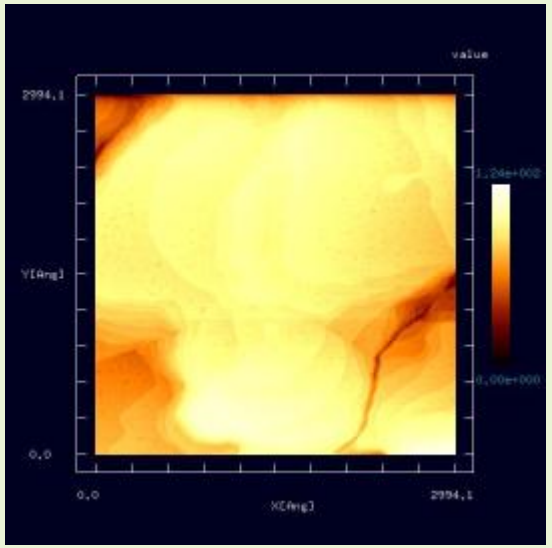
Changing the original image into a black-and-white image using the threshold value you set (from 0.0 and 1.0)



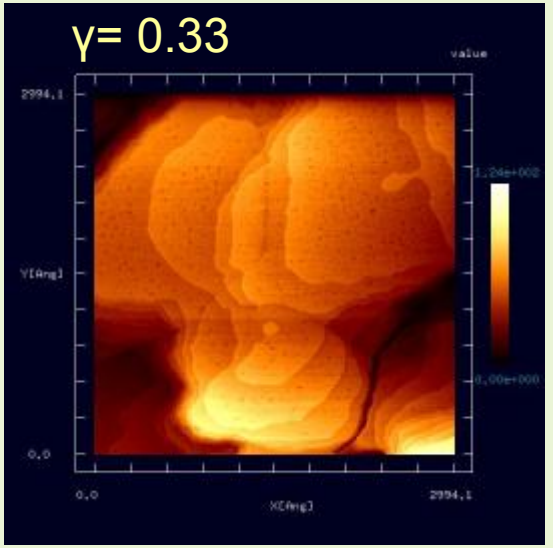


(The original image is provided by Professor Hiroyuki Hirayama, Nano-Quantum Physics at Surfaces and Interfaces, Department of Materials and Engineering, Tokyo Institute of Technology.)

Contrast adjustment (Gamma correction)



You set γ value (0.25~4.0)

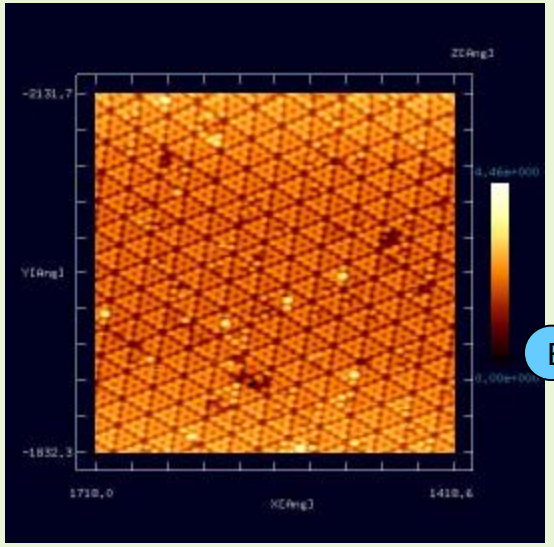


(The original image is provided by Professor Ken-ichi Fukui, Surface/Interface Chemistry Group, Department of Materials Engineering Science, Osaka University.)

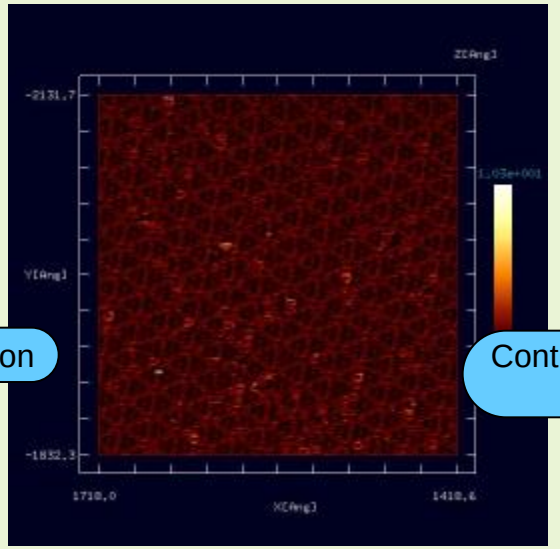
Digital Image Processings Function (2)

Analyzer

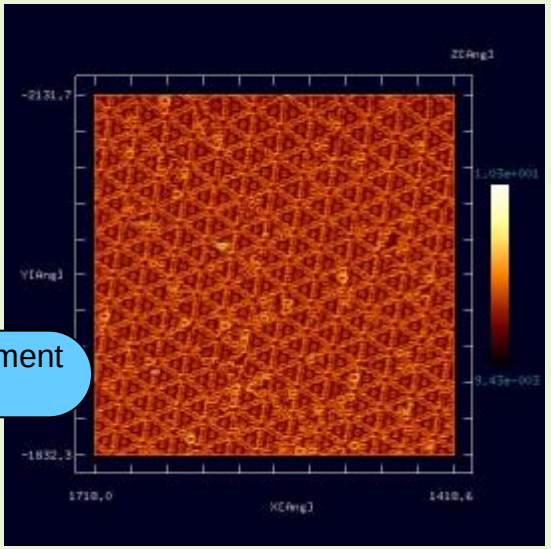
Edge detection with the Sobel filter



Edge detection

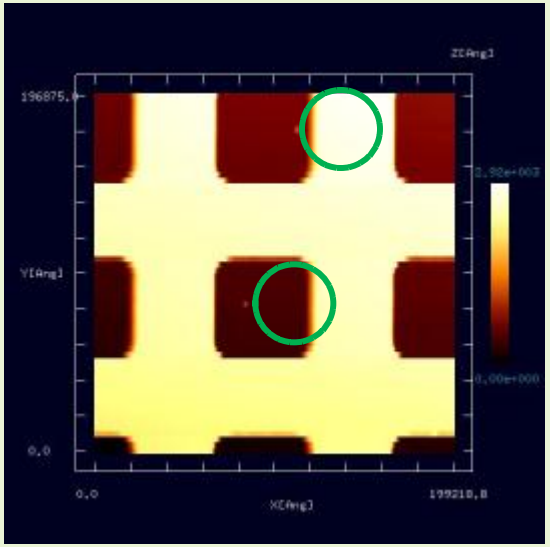


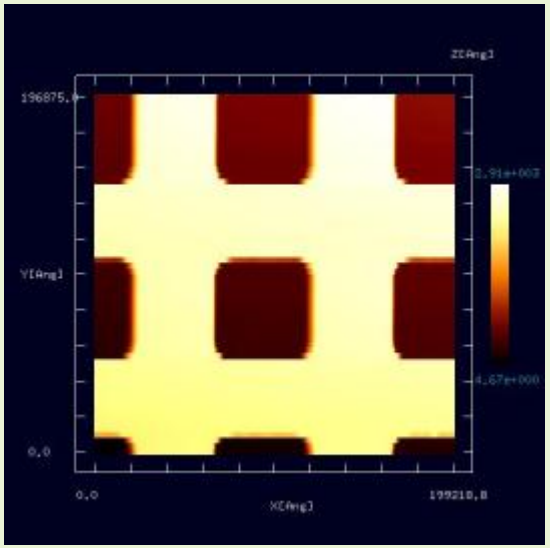
Contrast adjustment
γ=2.0



(The original image is provided by Professor Hiroyuki Hirayama, Nano-Quantum Physics at Surfaces and Interfaces, Department of Materials and Engineering, Tokyo Institute of Technology.)

Noise reduction with the median filter



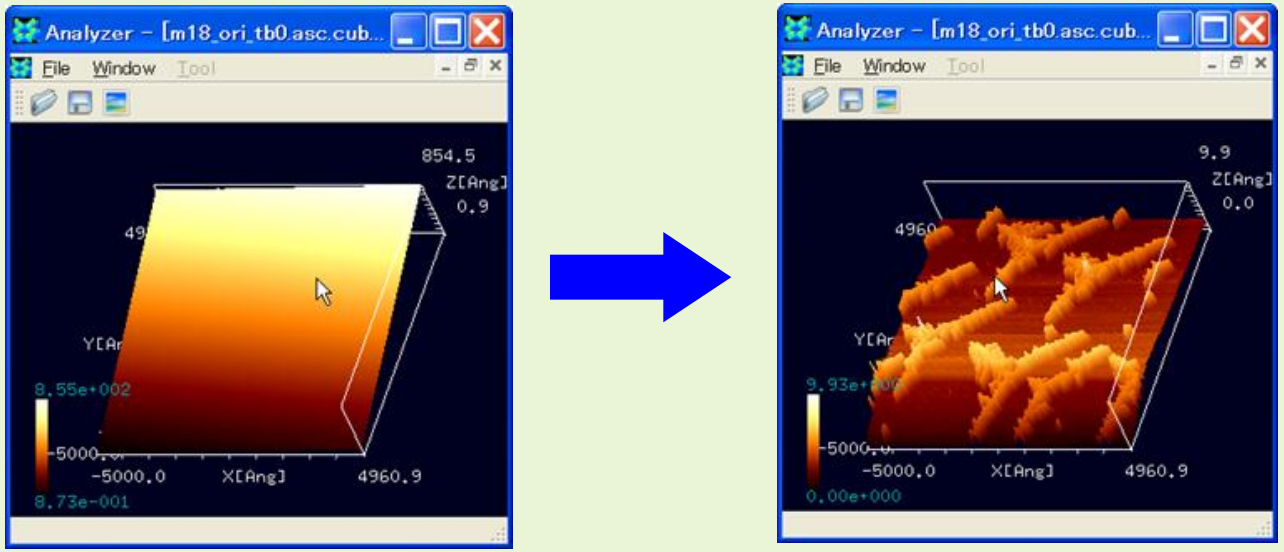


(The image is provided by Professor Katsushi Hashimoto, Solid-State Quantum Transport Group, Department of Physics, Graduate School of Science, Tohoku University.)

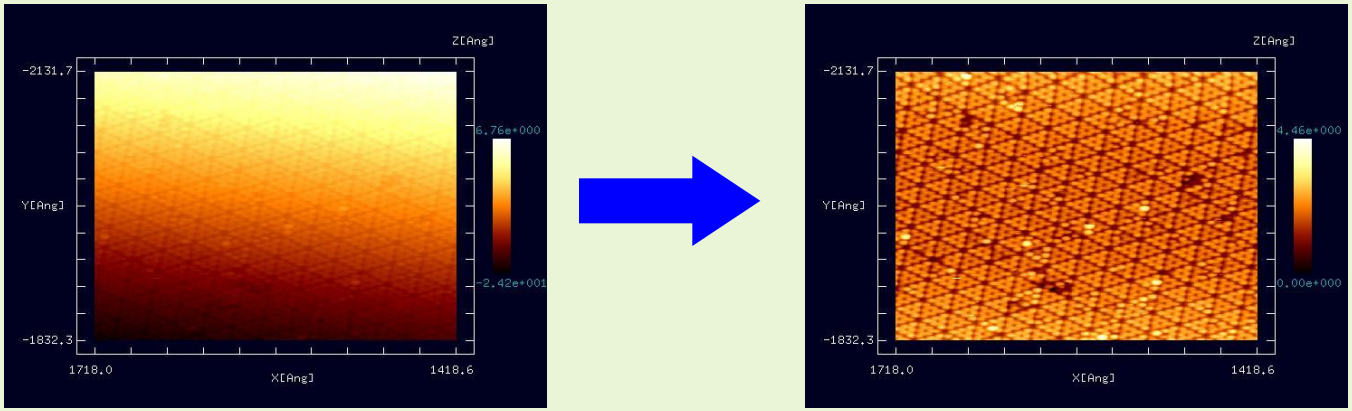
Digital Image Processings Function (3)

Analyzer

Correcting a tilt



(The original image is provided by the laboratory of the Professor Fukutani, Institute of Industrial Science, the University of Tokyo.)

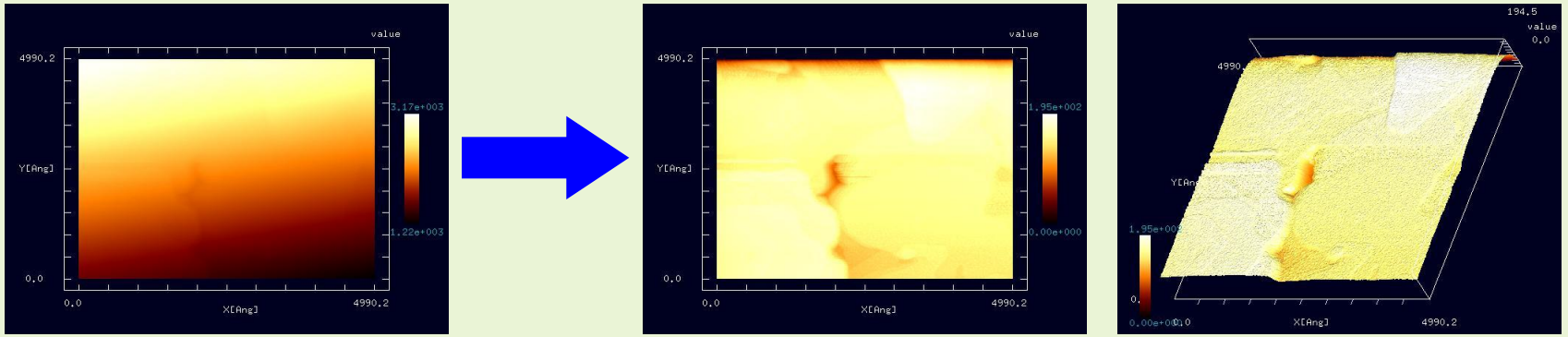


(The original image is provided by the laboratory of the Professor Hiroyuki Hirayama, Nano-Quantum Physics at Surfaces & Interfaces, Department of Materials & Engineering, Tokyo Institute of Technology.)

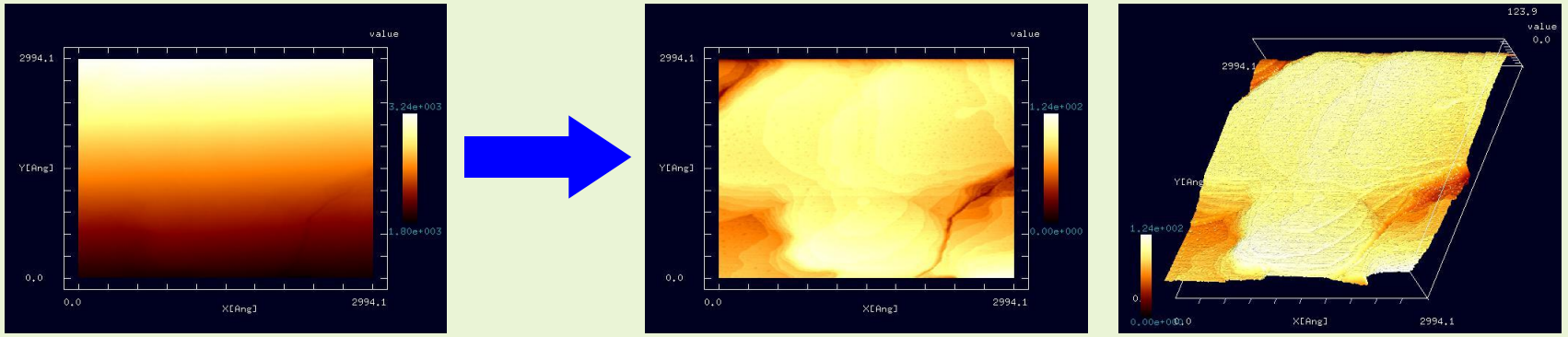
Digital Image Processings Function (4)

Analyzer

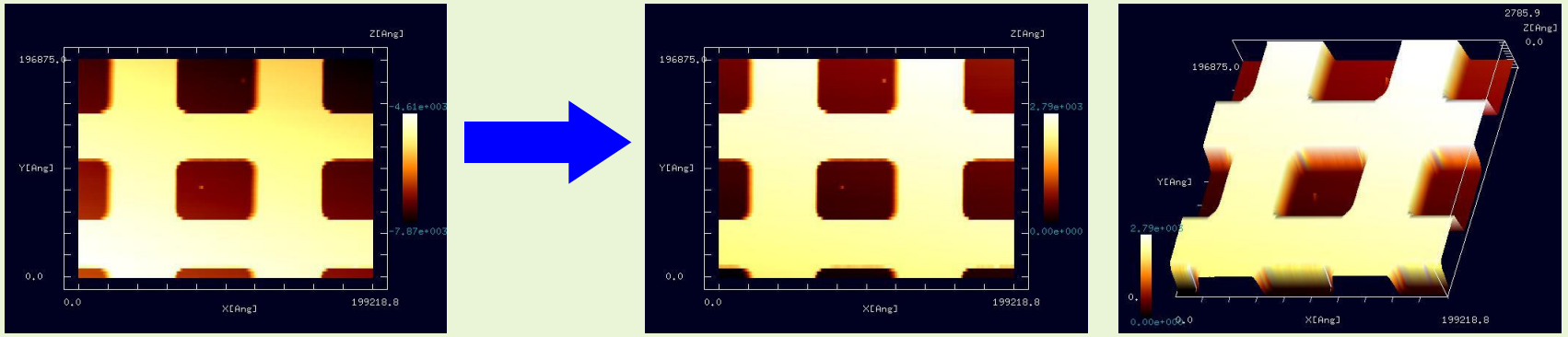
Correcting a tilt



(The original image is provided by Professor Ken-ichi Fukui, Division of Chemistry, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University.)



(The original image is provided by Professor Ken-ichi Fukui, Division of Chemistry, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University.)

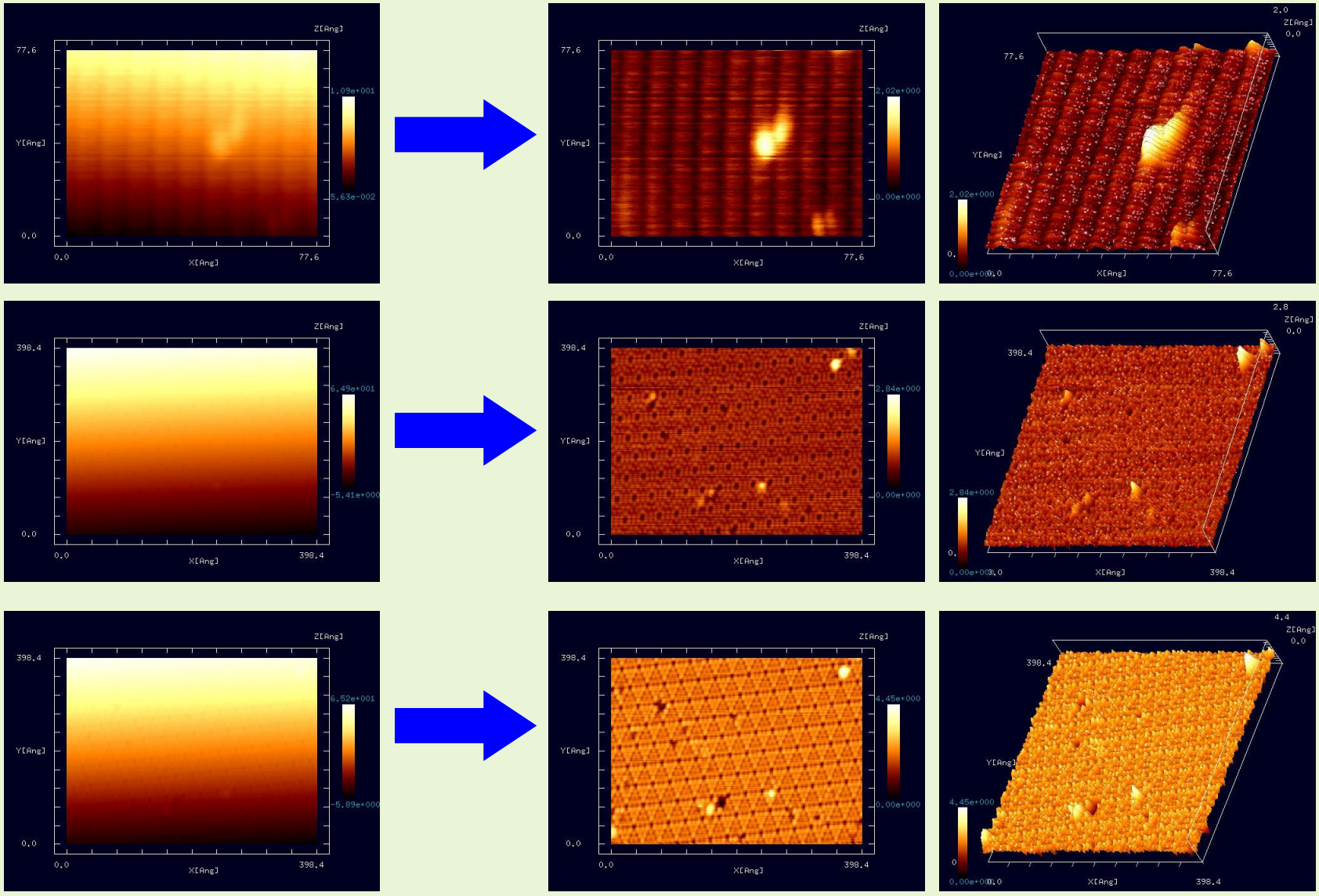


(The original image is provided by Dr. Katsushi Hashimoto, Solid-State Quantum Transport Group, Department of Physics, Tohoku University.)

Digital Image Processings Function (5)

Analyzer

Correcting a tilt



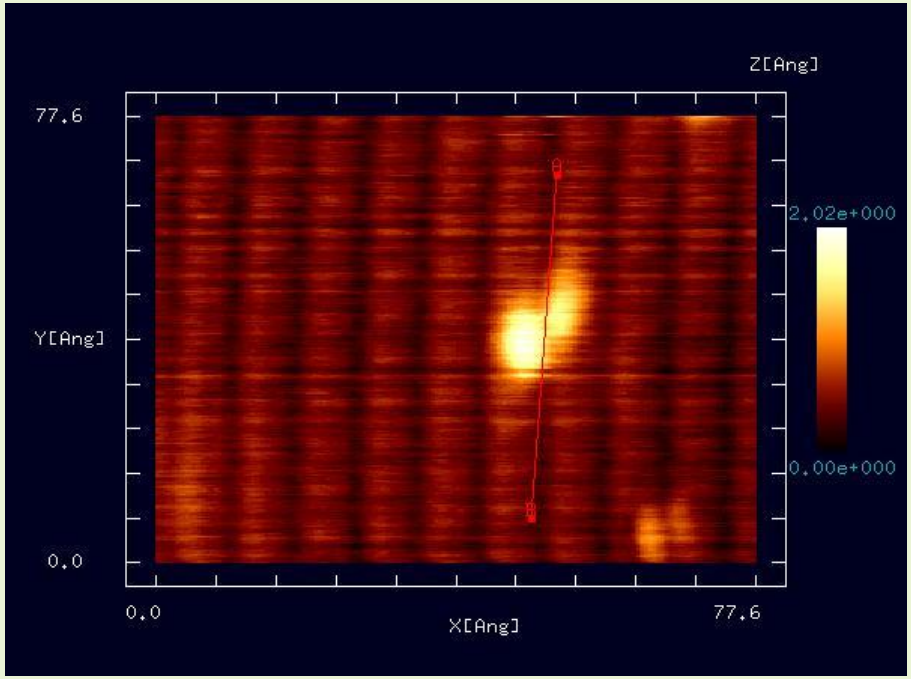
(The original image is provided by Professor Katsuyuki Fukutani, Vacuum and Surface Physics, Institute of Industrial Science, The University of Tokyo.)

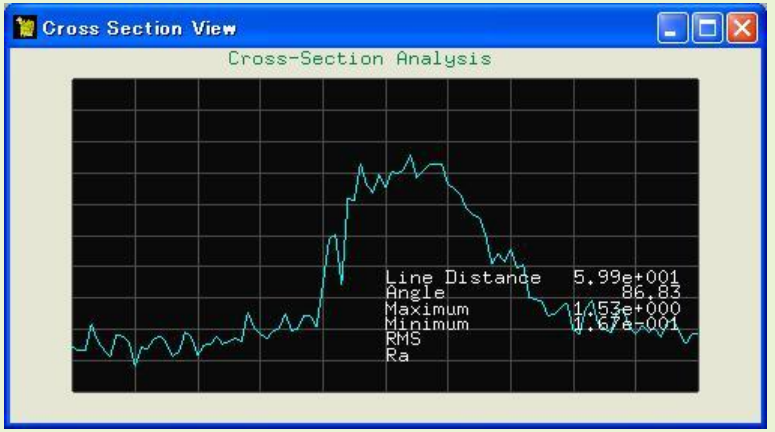
(The original image is provided by Professor Katsuyuki Fukutani, Vacuum and Surface Physics, Institute of Industrial Science, The University of Tokyo.)

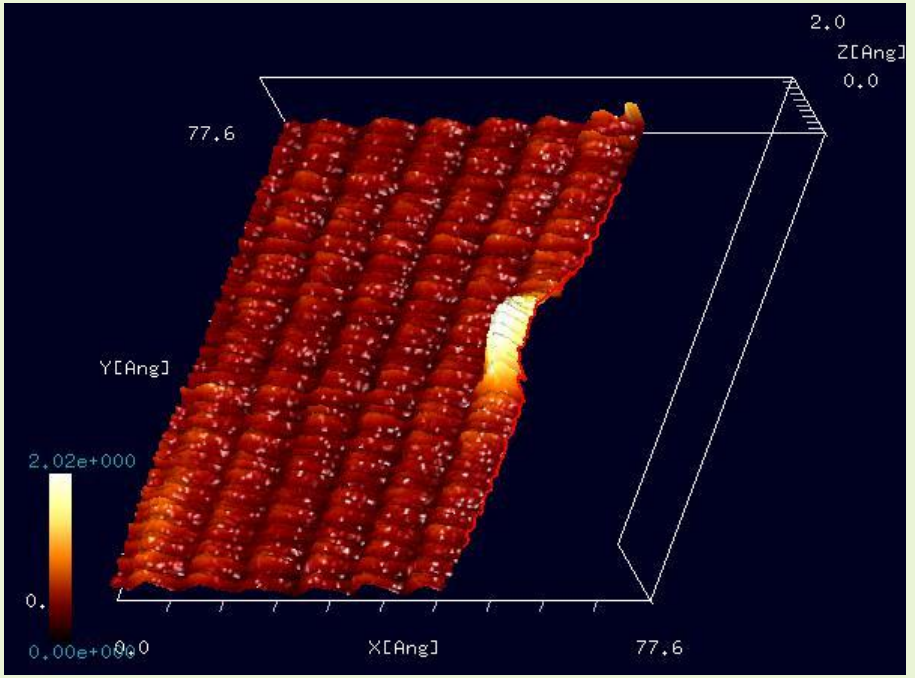
(The original image is provided by Professor Katsuyuki Fukutani, Vacuum and Surface Physics, Institute of Industrial Science, The University of Tokyo.)

Display the cross section

Display the cross section



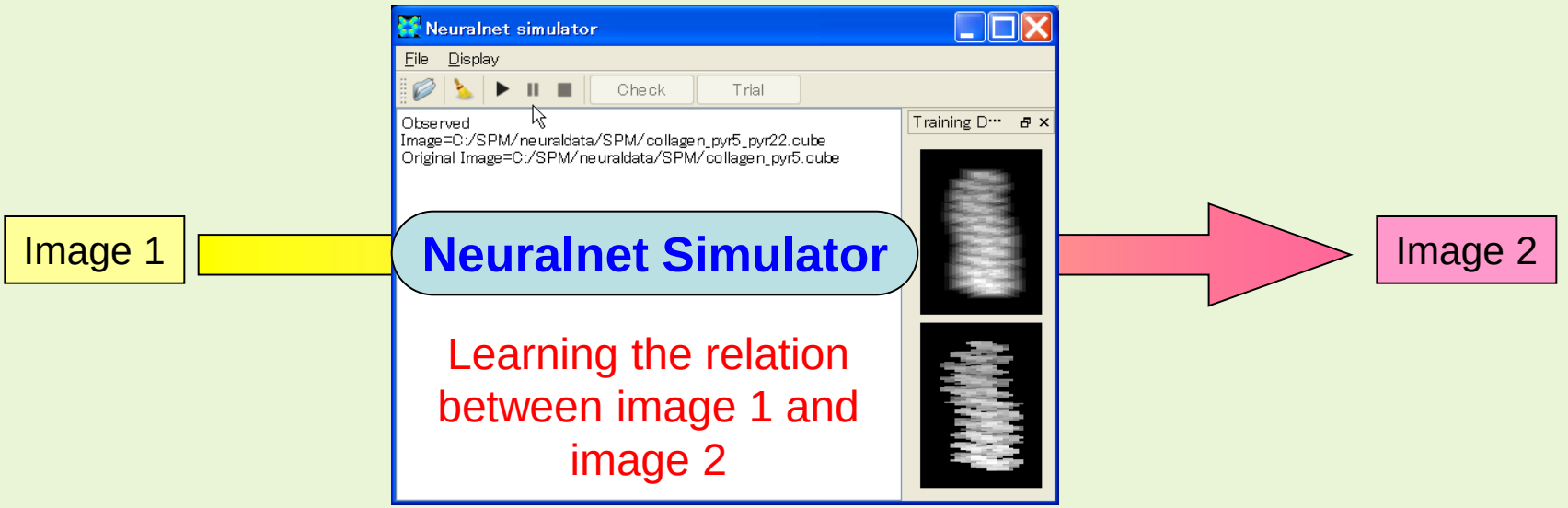




(The original image is provided by Professor Katsuyuki Fukutani, Vacuum and Surface Physics, Institute of Industrial Science, The University of Tokyo.)

Neural Network Simulator

Analyzer

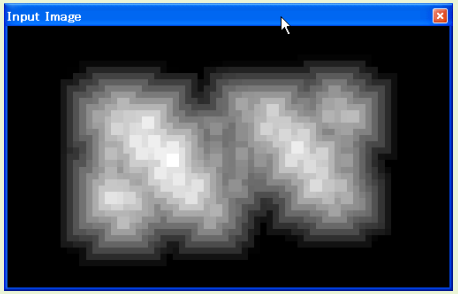


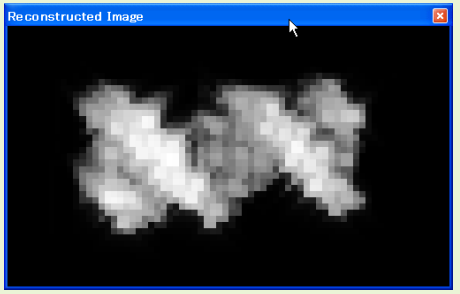
Observation process: The sample → The tip → The SPM image

Learning process: The SPM image of the known sample → Neural network → The known sample

Applying the results of the learning

Estimating process: The SPM image of any sample → Neural network → The estimated sample



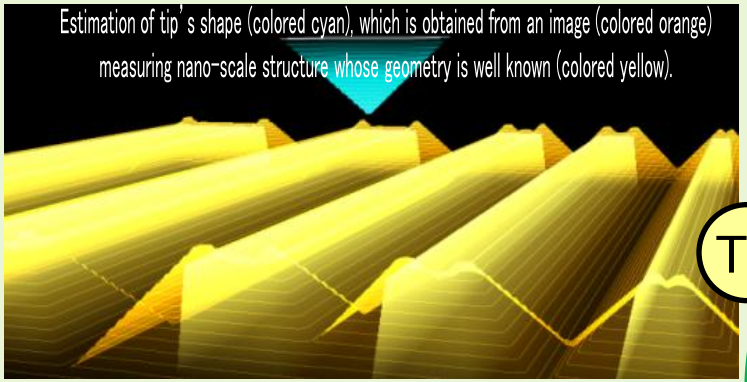


We can obtain the image from which the artifacts are removed.

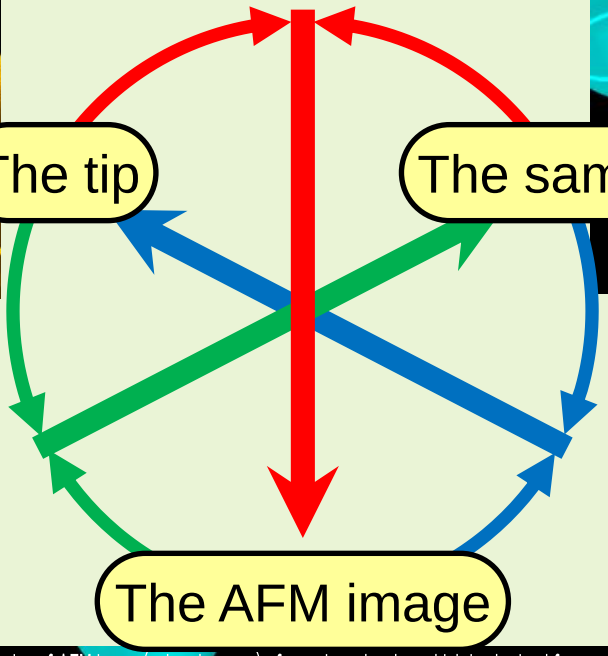
GeoAFM

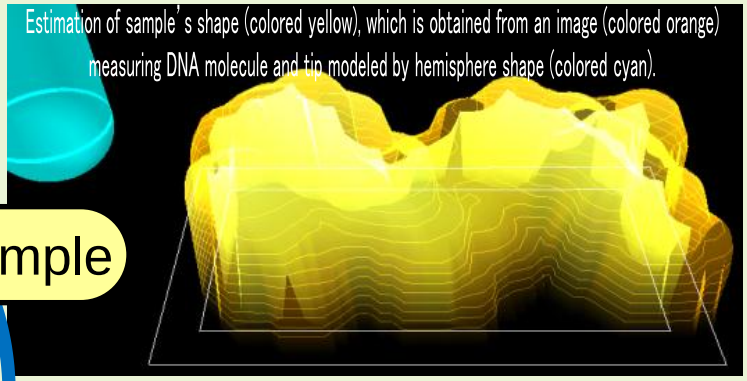
Geometrical Mutual AFM Simulator

Geometrical Mutual AFM Simulator (GeoAFM) provides users with a kind of a three-way data processor, so that it reconstructs the one out of the other two among three geometrical elements, a tip, a sample material and its AFM image. The GeoAFM produces a result from only the information of the geometry of the tip, the sample material and the AFM image.

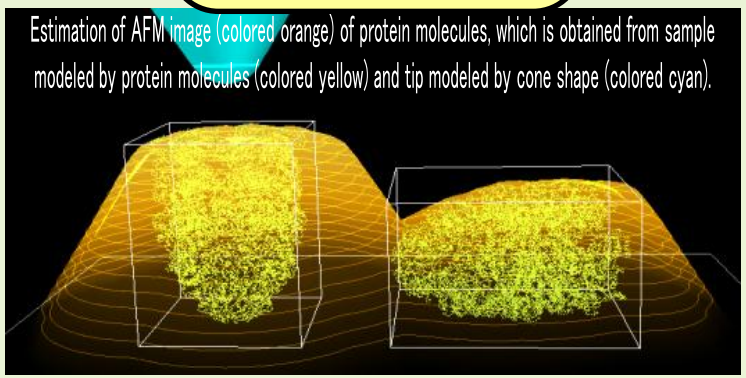


Estimation of Tip's shape from sample's structure and its image.





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



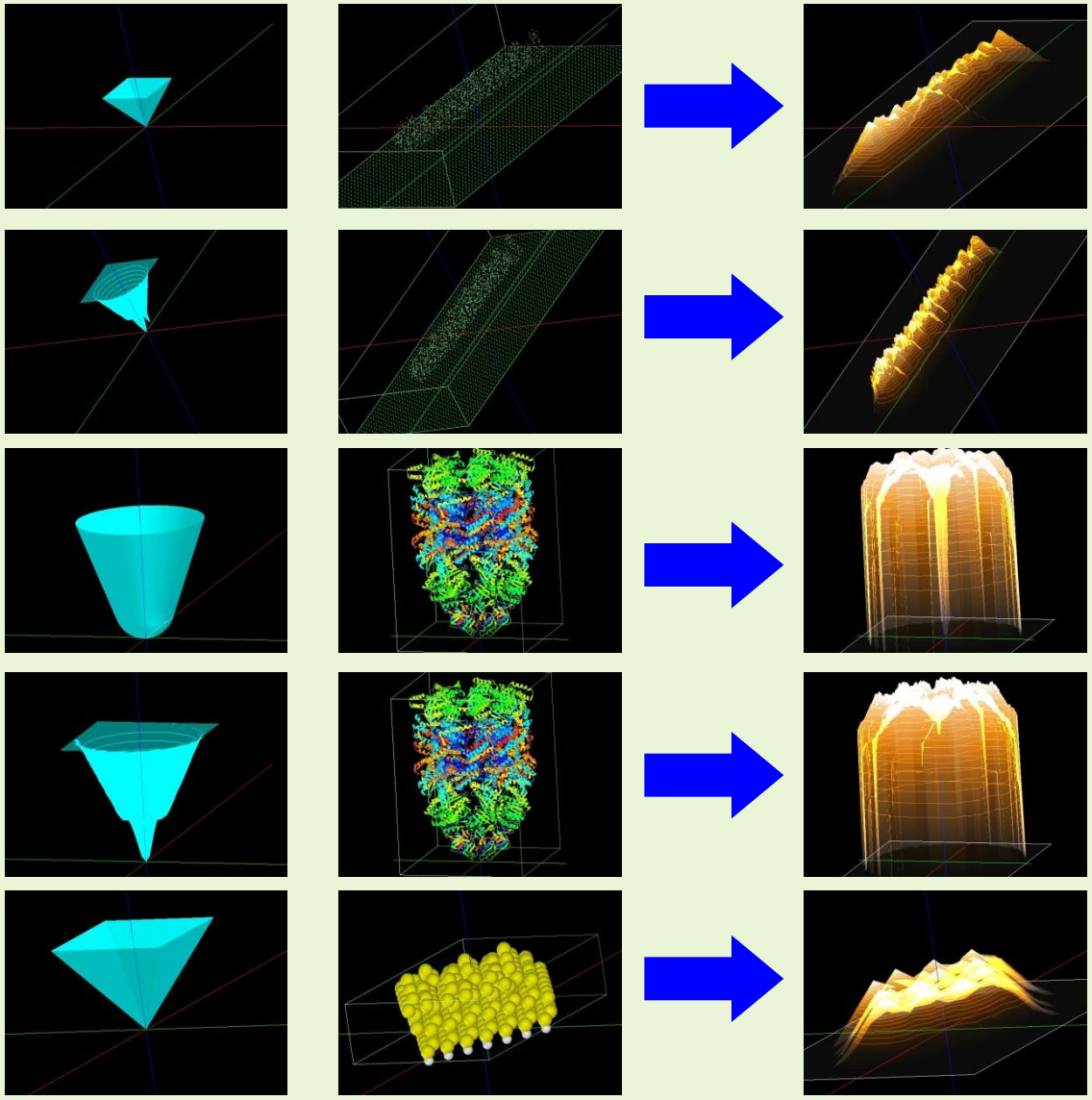
Estimation of AFM Image from tip model and sample model.

Geometrical Mutual AFM Simulator

GeoAFM

Estimation of AFM Image from tip model and sample model.

The tip | The sample | The AFM image



•Simulation of the AFM image of a Glycoprotein (1clg) on HOPG (Highly Oriented Pyrolytic Graphite) by the use of a quadrilateral pyramid probe tip.

•Simulation of the AFM image of a Glycoprotein (1clg) on HOPG (Highly Oriented Pyrolytic Graphite) by the use of a broken double tip.

•Simulation of the AFM image of a GroEL (chaperonin) by the use of a cone probe tip. The chaperonin is a basket-shaped polymer of 140 Å width, 140 Å depth and 200 Å height. The simulated AFM image reproduces a hole on the top of the basket shape.

•Simulation of the AFM image of a GroEL (chaperonin) by the use of a broken double tip. The chaperonin is a basket-shaped polymer of 140 Å width, 140 Å depth and 200 Å height. The simulated AFM image reproduces a hole on the top of the basket shape.

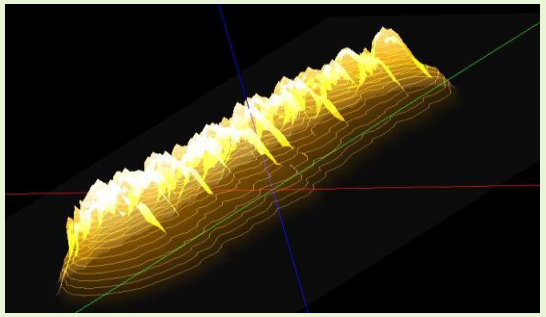
•Simulation of the AFM image of a Si(111)-(7x7) DAS surface by the use of a quadrilateral pyramid probe tip.

GeoAFM

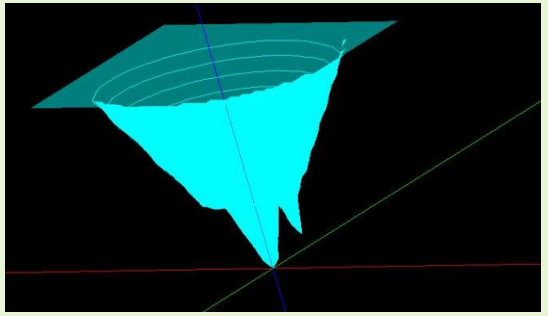
Geometrical Mutual AFM Simulator

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

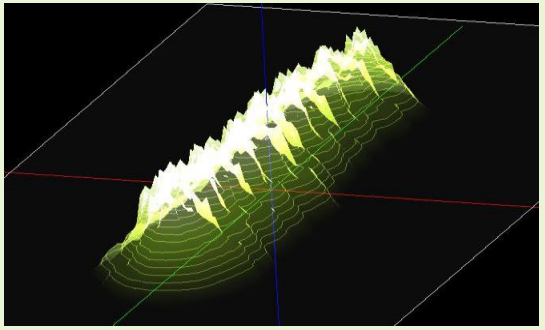
The AFM image



The tip



The sample



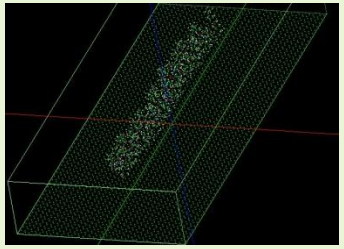
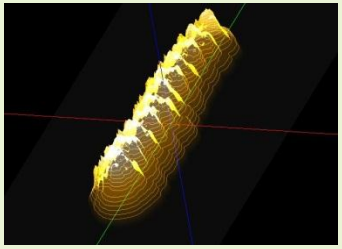
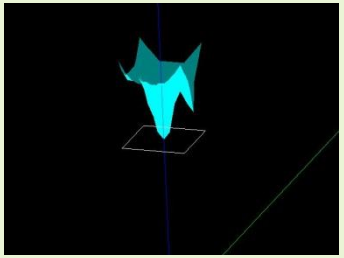
•Simulation of the sample surface by removing the artifacts from an AFM image of a Glycoprotein (1clg) on HOPG (Highly Oriented Pyrolytic Graphite) by the use of a broken double tip.

GeoAFM

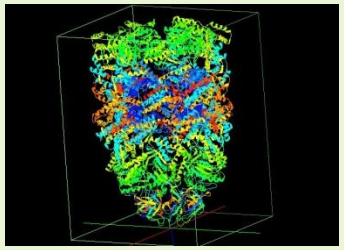
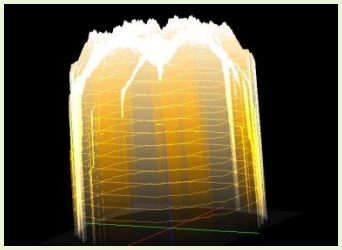
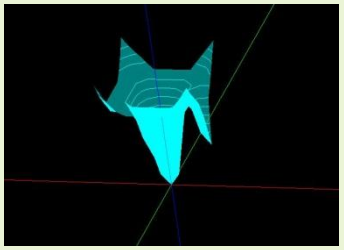
Geometrical Mutual AFM Simulator

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

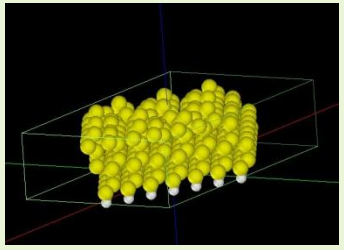
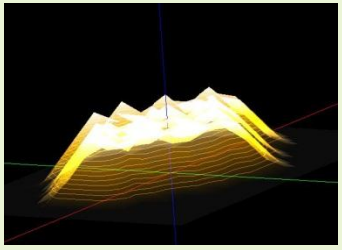
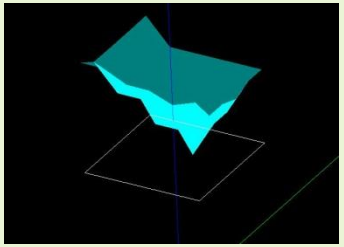
The sample | The AFM image → The tip

•Simulation of the tip shape from an AFM image of a Glycoprotein (1clg) on HOPG (Highly Oriented Pyrolytic Graphite) by the use of a broken double tip, and from a sample surface data constructed by a molecule structure.

•Simulation of the tip shape from an AFM image of a GroEL (chaperonin) by the use of a broken double tip, and from a sample surface data constructed by a molecule structure. The chaperonin is a basket-shaped polymer of 140 Å width, 140 Å depth and 200 Å height.

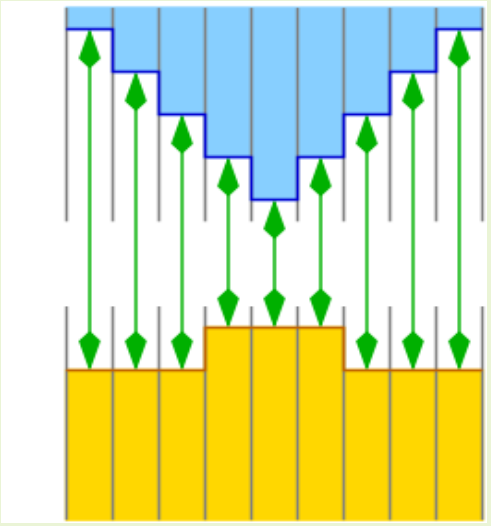
•Simulation of the tip shape from an AFM image of a Si(111)-(7x7) DAS surface, and from a sample surface data constructed by the atomic structure of a crystal surface.

The Comparison between Normal method and GeoAFM

Calculation by
Interaction force
2 weeks by a WS

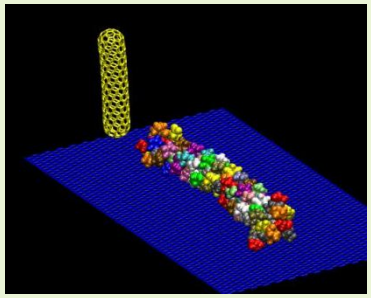
Calculation by
Geometrical condition
1 second by a PC

Rapid geometrical method



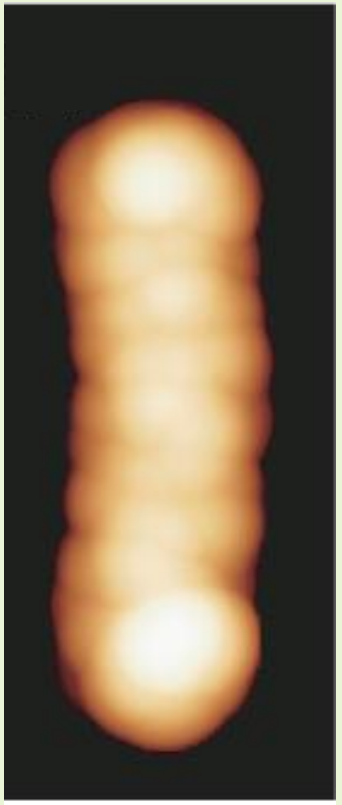
MD

GeoAFM



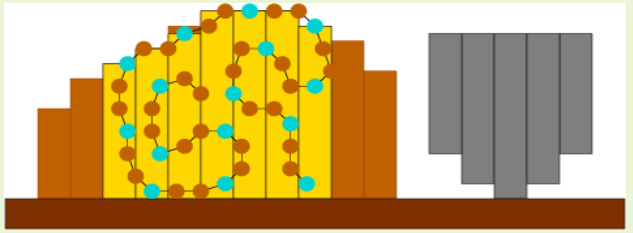
Geo AFM reproduces an AFM image observed by an experiment well.

The tip recognize the difference in height of the Pro and the Gly.



Collagen image

By 2 x 10^{-8} shorter !!

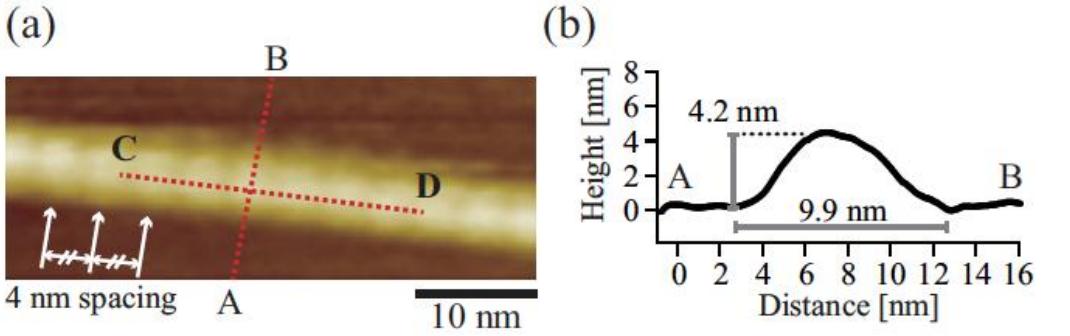


Divide tip/sample into meshes assign the height of each mesh by the top atom, and measure the difference in height. It is a geometrical method, so the computational complexity is little.

FM-AFM observation and AFM simulation of tubulin in liquid

H.Asakawa, K.Ikegami, M.Setou, N.Watanabe, M.Tsukada, T.Fukuma.
Biophysical Journal 101(5), 1270-1276 (2011).

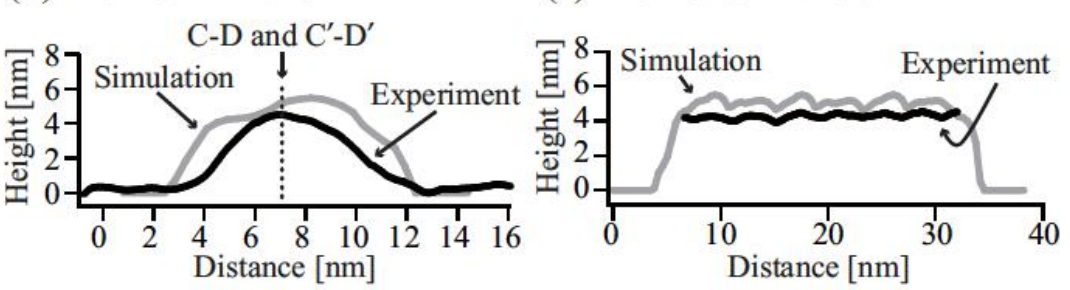
Experimental AFM image



Simulated AFM image

GeoAFM

The Comparison between the Experimental Image and Simulated Image



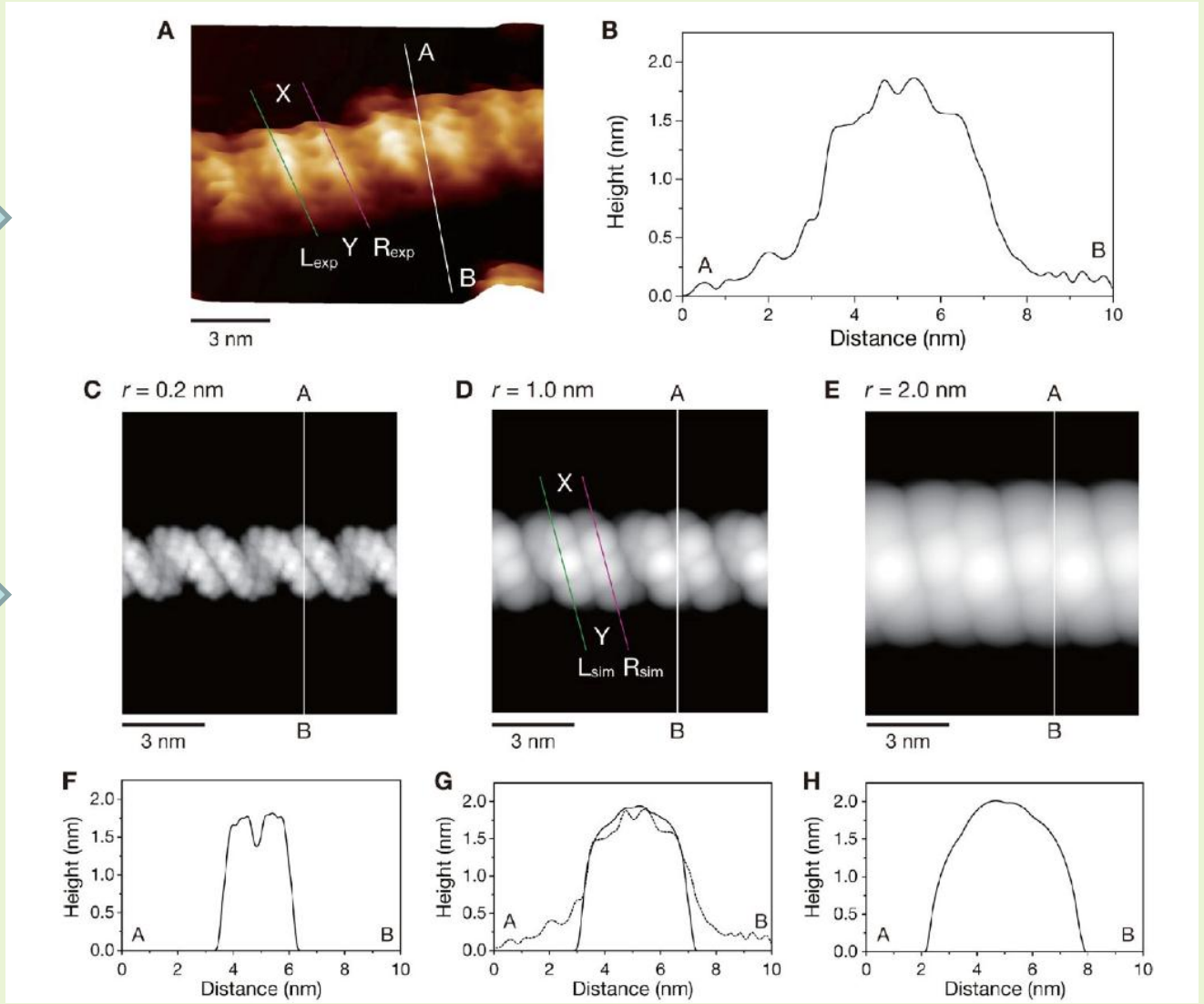
Direct observation and Simulation of the DNA in aqueous solution

S. Ido, K. Kimura, N. Oyabu, K. Kobayashi, M. Tsukada, K. Matsushige and H. Yamada, ACS Nano 7(2), 1817-1822 (2013). DOI: 10.1021/nn400071n

FM-AFM experiments

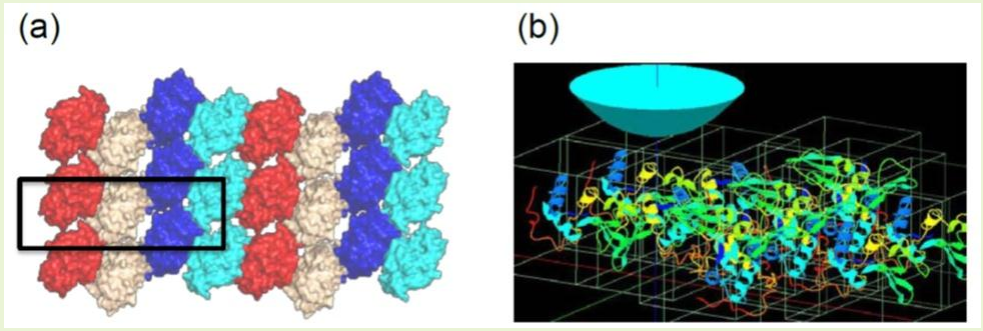
The theoretical simulation

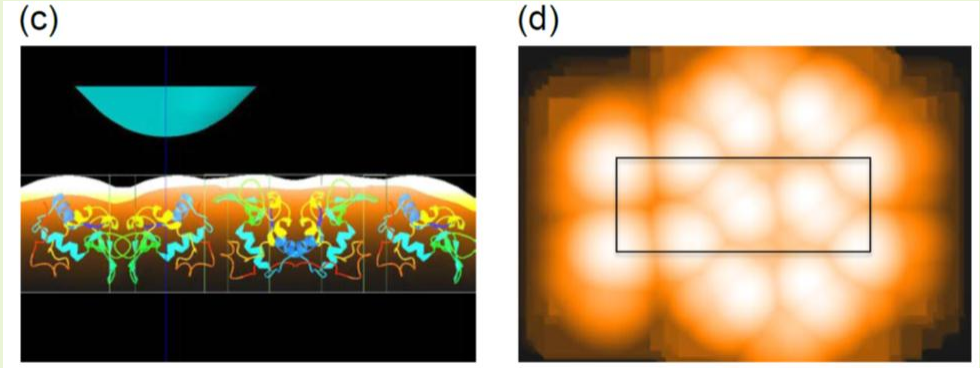
GeoAFM



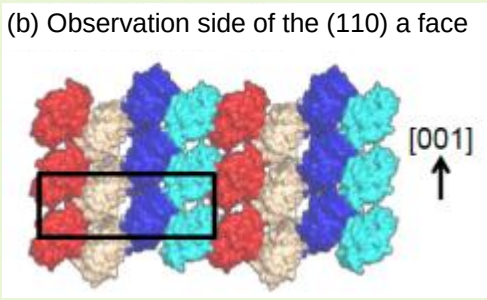
Decision of the (110) face of tetragonal lysozyme single crystal in liquid

The (110) face of tetragonal lysozyme single crystal has two possibilities that the surface structure is a (110) a face or a (110) b face.





Creation of the SPM simulator image



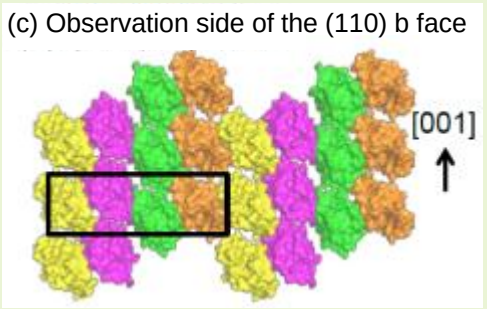
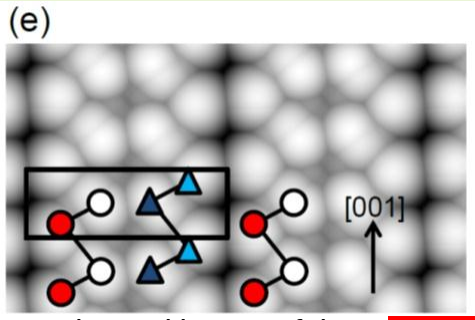
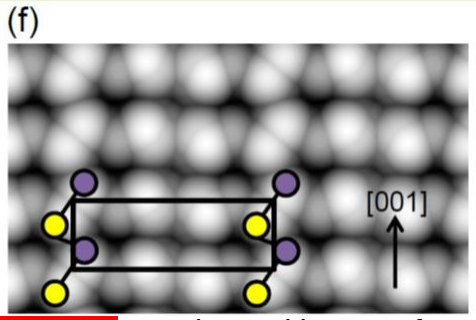


Diagram of the crystal structure of tetragonal lysozyme



Estimated image of the (110) a face

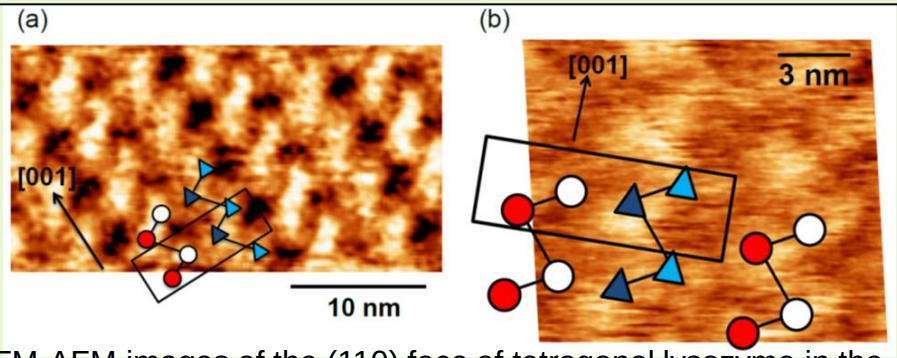
GeoAFM



Estimated image of the (110) b face

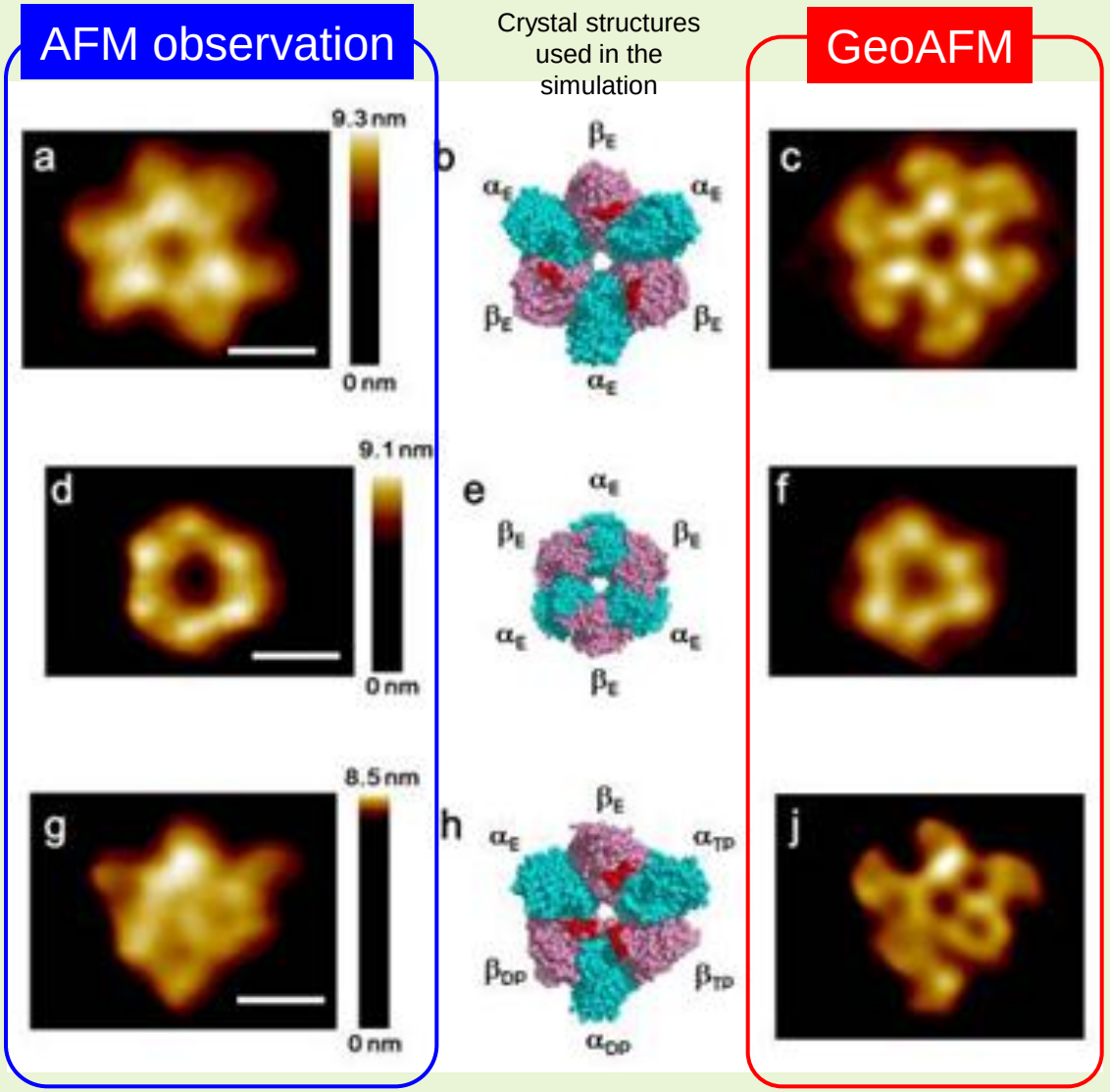
Comparing between the observed AFM image and the simulated image, the (110) face of tetragonal lysozyme single crystal is a (110)a surface structure.

(The original images are provided by Assistant Professor Ken Nagashima, Phase Transition Dynamics Group, Frontier Ice and Snow Science Division, Institute of Low Temperature Science, Hokkaido University)



FM-AFM images of the (110) face of tetragonal lysozyme in the solution (actual survey)

AFM observation and simulation of rotating molecular motor F_1-ATPase



Agree well

F_1-ATPase:

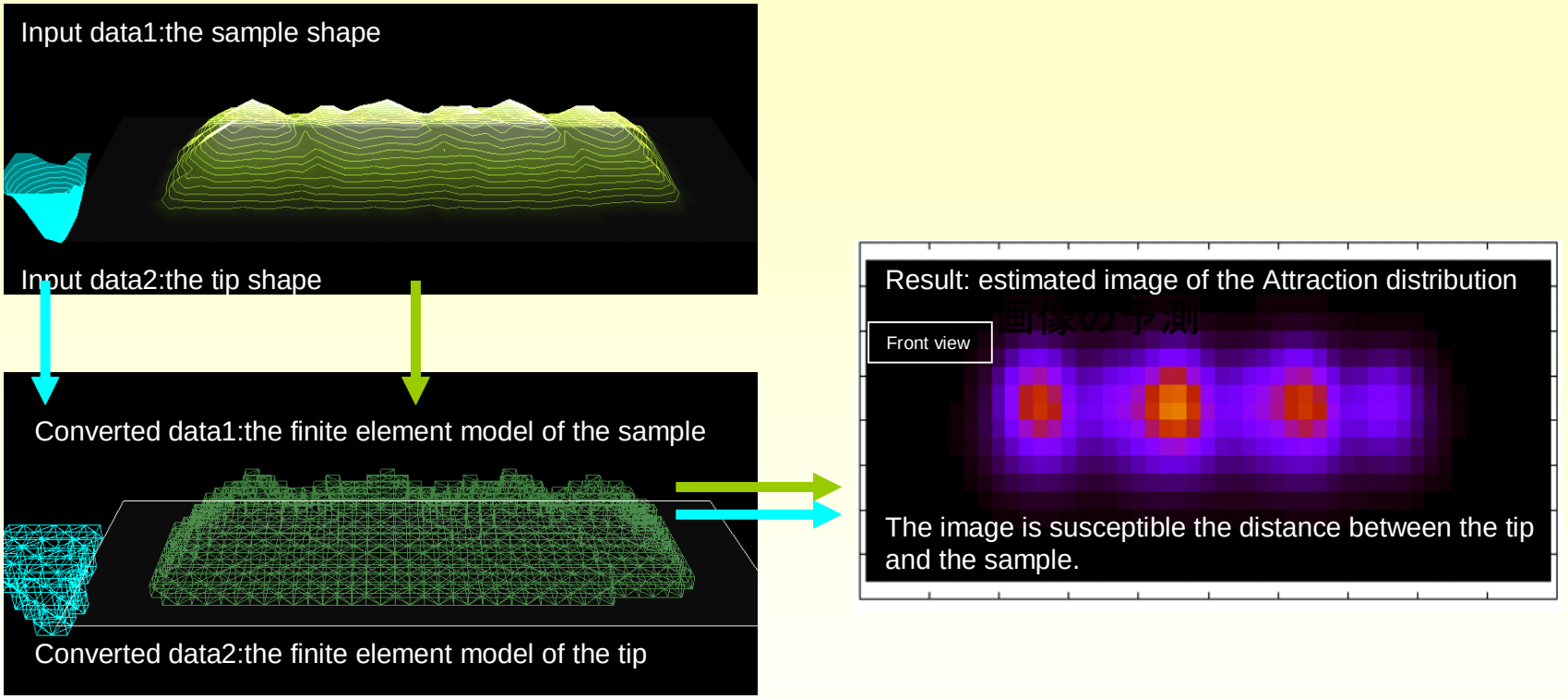
The rotary moleculer motor which turns a subunit using hydrolysis energy of the ATP in one direction.

The Comparison between the observed and the simulated images corroborated the reliability of the experiment.

(The original images are provided by Associate Professor takayuki Uchibashi, Kanazawa Biophysics Lab, Department of Physics, Bio-AFM Frontier Research Center, Kanazawa University)

Estimation of the measured image which was deformed by the interaction from the sample model.

FemAFM

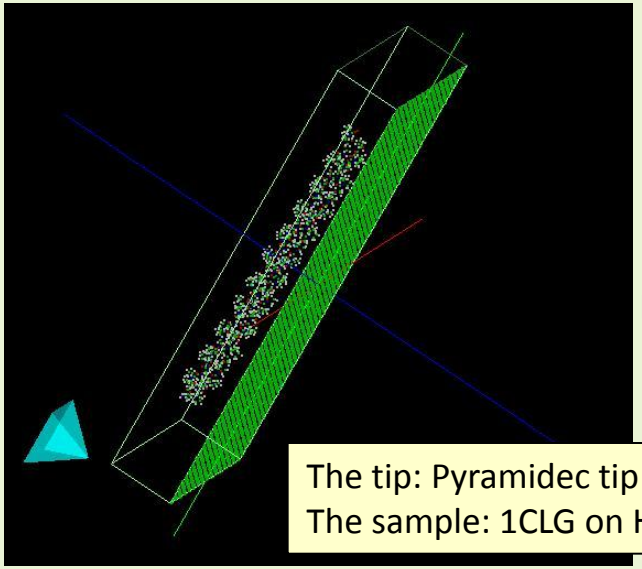


Convert shape of the tips and the samples into continuum of the finite element which have the modulus of elasticity and the van der Waals force.
Calculate the interaction and the elastic deformation.
Imaging the attraction distribution suffered by the tip.

Finite element method AFM simulator (FemAFM) simulates the AFM image using the finite element method.
It is different from Geometrical Mutual AFM Simulator (GeoAFM), it treats a deformation of the shape of the sample and the tip.

An AFM simulation of a single molecule of Glycoprotein (1clg)

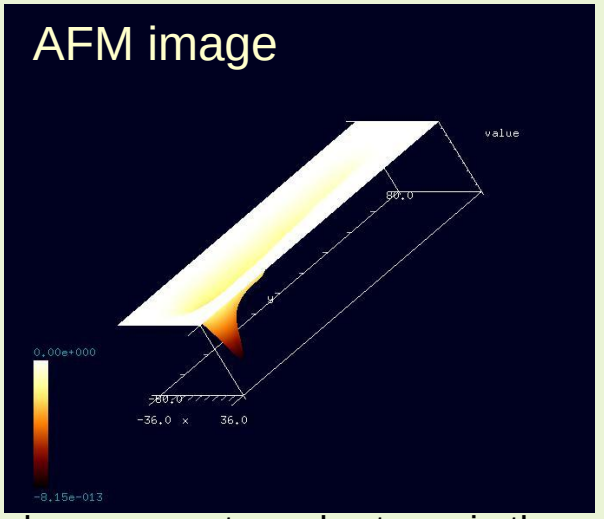
FemAFM



The tip: Pyramidec tip (SiO_2)
The sample: 1CLG on HOPG

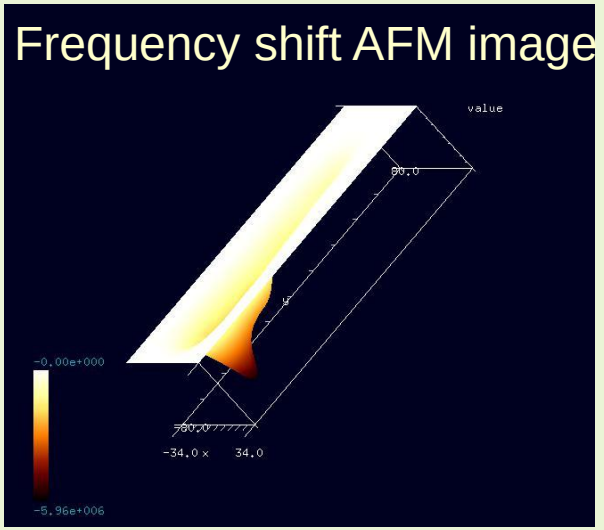
HOPG: Highly Oriented Pyrolytic Graphite
1CLG:Glycoprotein(CLG：ε-caprolacton・(L)lactide・glycolide copolymer)

Non-contact mode



The van der Waals force becomes extremely strong in the area where the tip is quite close to the sample surface, due to the law of inverse power of six.

Femafm_frequency_ shift mode

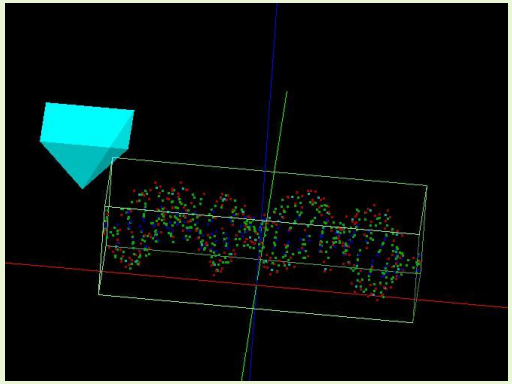


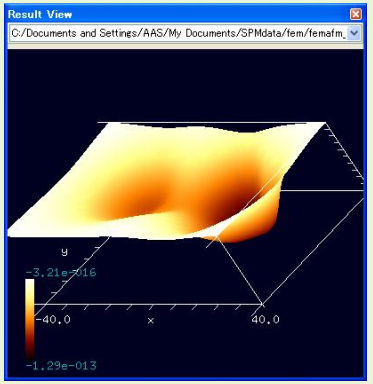
The cantilever oscillates at 500[MHz]. The maximum value of the frequency shift is about 5.96[MHz].

FemAFM

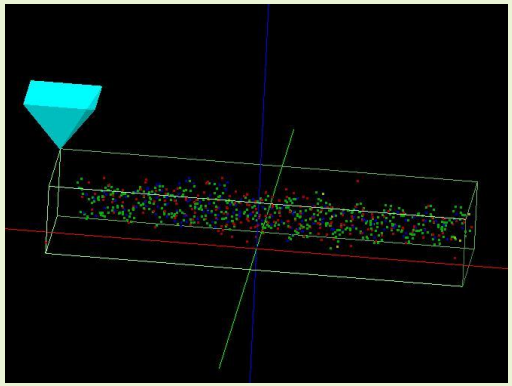
Non-contact mode

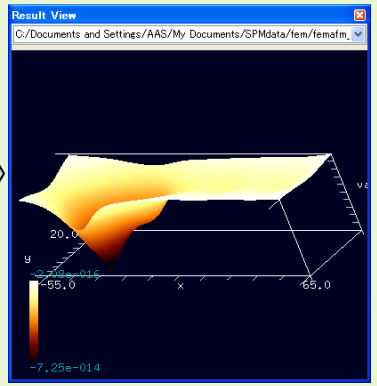
A probe tip attached to the front edge of the cantilever scans the surface of the sample material, keeping the distance around a few angstroms.



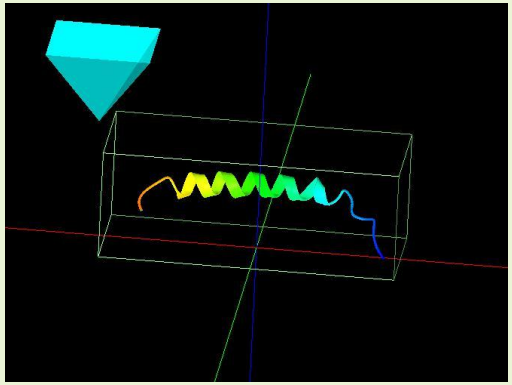


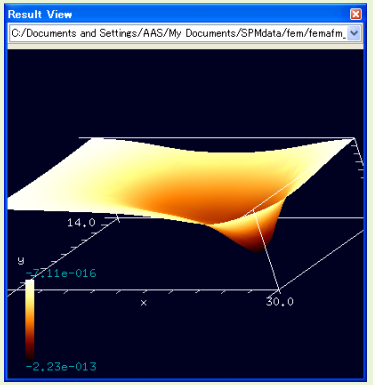
•Simulation of the AFM image of a DNA (Self-assembled Three-Dimensional DNA).





•Simulation of the AFM image of a collagen (collagen alpha-1(III) chain).



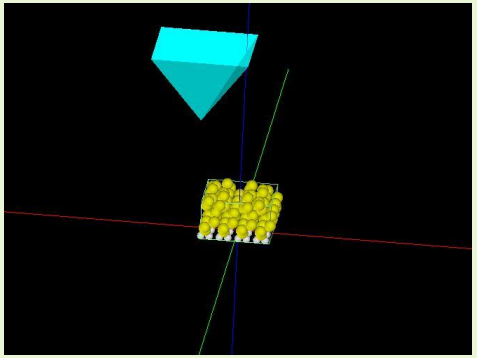


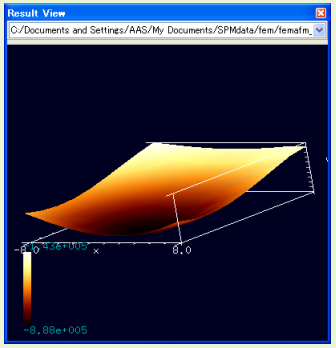
•Simulation of the AFM image of a collagen (COLLAGEN ALPHA 1).

FemAFM

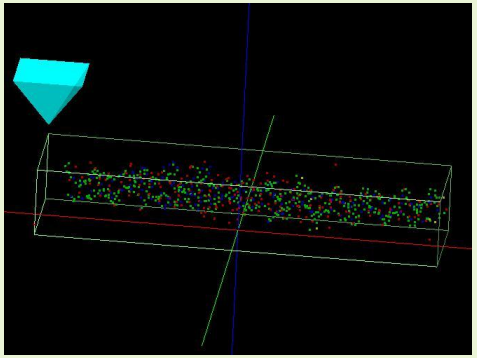
Frequency shift image mode

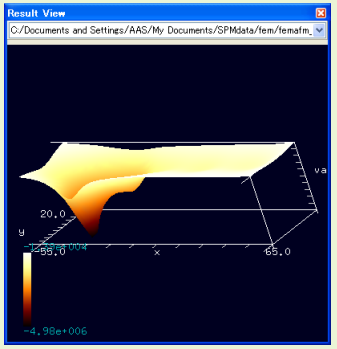
A cantilever, which is oscillated by an external force with a constant frequency, approaches a sample surface but does not contact with it. A frequency shift caused by an interaction between a tip and a sample is calculated.



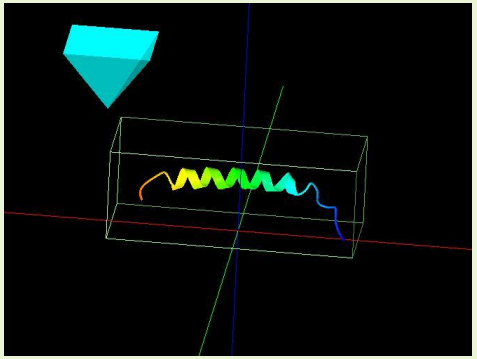


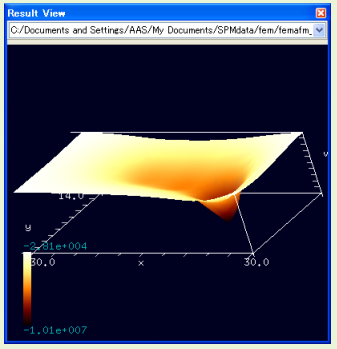
•Simulation of the frequency shift AFM image of a Si(111)-(7x7) DAS surface.





•Simulation of the frequency shift AFM image of a collagen (collagen alpha-1(III) chain).



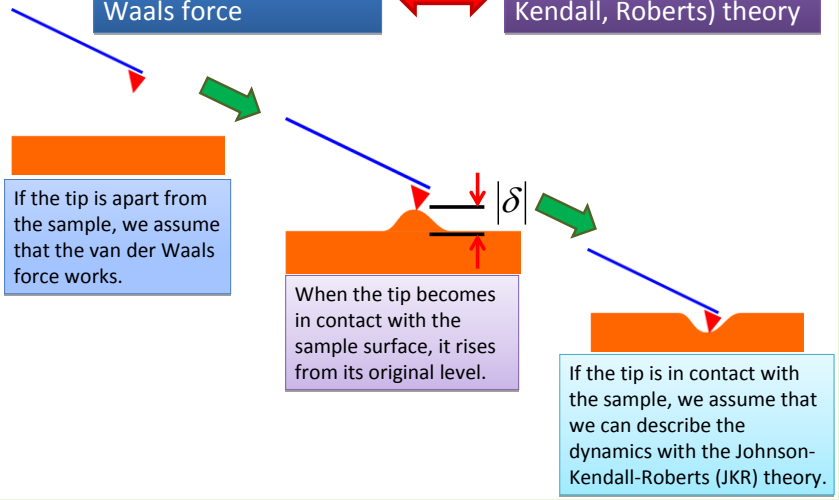


•Simulation of the frequency shift AFM image of a collagen (COLLAGEN ALPHA 1).

Principle of a Method for Investigating Viscoelastic Contact Analysis

Model of the visoelastic contact between the tip and the sample

Model of the van der Waals force ⟷ The JKR (Johnson, Kendall, Roberts) theory

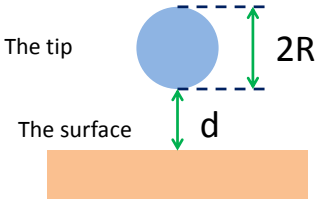


If the tip is apart from the sample, we assume that the van der Waals force works.

When the tip becomes in contact with the sample surface, it rises from its original level.

If the tip is in contact with the sample, we assume that we can describe the dynamics with the Johnson-Kendall-Roberts (JKR) theory.

Van der Waals force



$$F \cong \frac{A}{12}\frac{D}{d^2}$$

Where $D = 2R$, $A = \sqrt{H_1 H_2}$

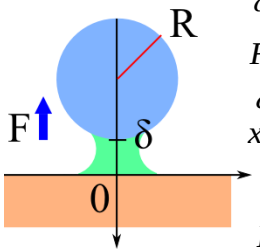
H_1 , H_2 :Hamaker constant

The tip ⟶ elastic body with no viscous characteristic

The sample ⟶ viscoelastic ➡ Introduction of surface tension

➡ We assume that the dynamics can be described by the JKR theory.

The JKR theory



F :The force between the tip and the sample. (It is positive in the vertical upward direction.)

δ :The length between the tip and the sample. (It is positive in the vertical downward direction.)

$$F = 4F_c(x^3 - x^{3/2})$$

$$\delta = \delta_0(3x^2 - 2\sqrt{x})$$

x :The dimensionless quantity which is in proportion to a contact area of the tip and the sample.

$$6^{-2/3} \le x \le 1$$

$F_c = 3\pi\gamma R$ (γ :surface tension of the sample)

$$\delta_0 = \frac{a_0^{\,2}}{3R}, \quad a_0 = \left(\frac{9\pi\gamma R^2}{E^*}\right)^{1/3}, \quad \frac{1}{E^*} = \frac{1-\sigma_1^{\,2}}{E_1} + \frac{1-\sigma_2^{\,2}}{E_2}$$

E_1 , E_2 Young's modulus σ_1 , σ_2 :Poisson's ratio

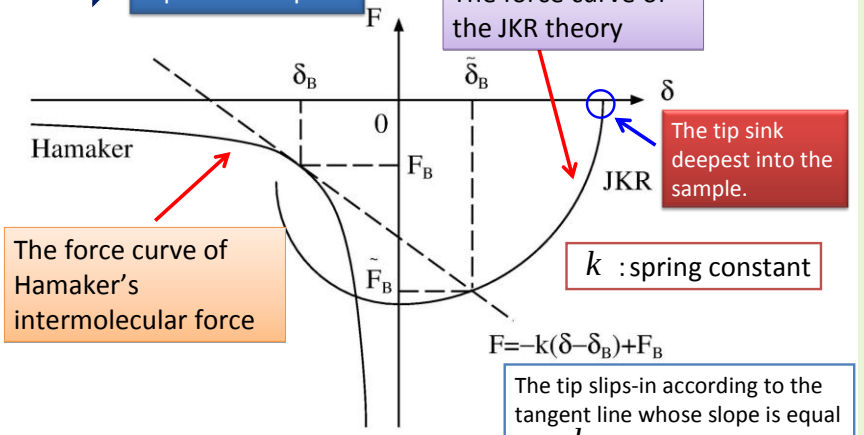
a_0 : The contact area at a zero load. When the tip goes down below the surface of the sample, and the adhesive force of the surface tension and the repulsive force of the elasticity cancel each other out with the tip, the area of their contact is equal to a_0.

$a = a_0 x$:contact area

Transition between a state where van der Waals force works and a state where the JKR theory is effective.

Slip-in and Slip-out

The force curve of the JKR theory



The tip sink deepest into the sample.

The force curve of Hamaker's intermolecular force

k :spring constant

The tip slips-in according to the tangent line whose slope is equal to $-k$.

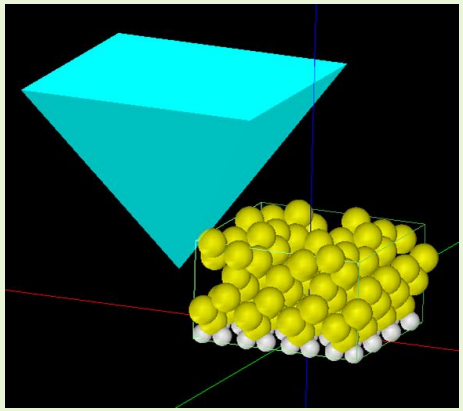
Transition from the theory of van der Waals force to the JKR theory

A Method for Investigating Viscoelastic Contact Analysis

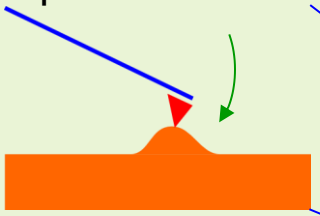
FemAFM

A Method for Investigating Viscoelastic Contact Analysis Mode

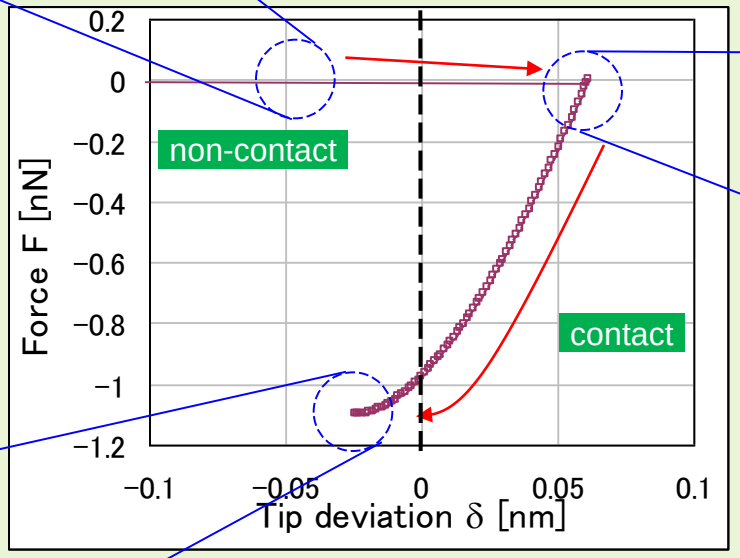
We let a cantilever vibrate at constant frequency by external force. We can simulate successive processes such as making the tip become in contact with the sample surface, making the tip be stuck with the sample by the adhesive force, letting the tip be pushed back upwards outside the sample, and letting the tip leave the sample surface.



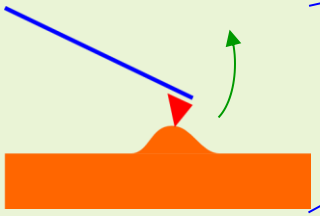
The tip: Pyramidec tip (SiO_2)
The sample: Si(001)



The tip came in contact with the sample above the surface.



The tip is pushed into the interior of the sample.

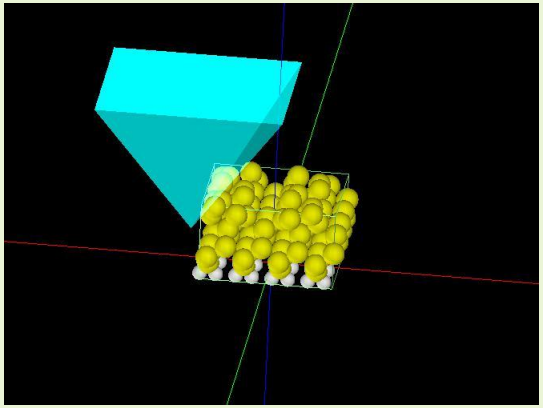


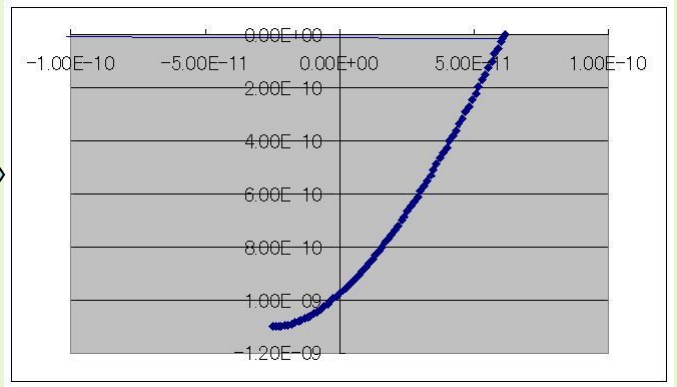
Till the tip leaves the sample.

Direction of the force that the tip experienced is positive in the vertical upward direction.

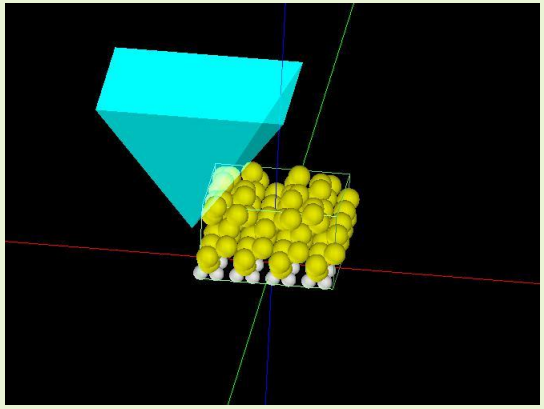
Viscoelastic dynamics mode

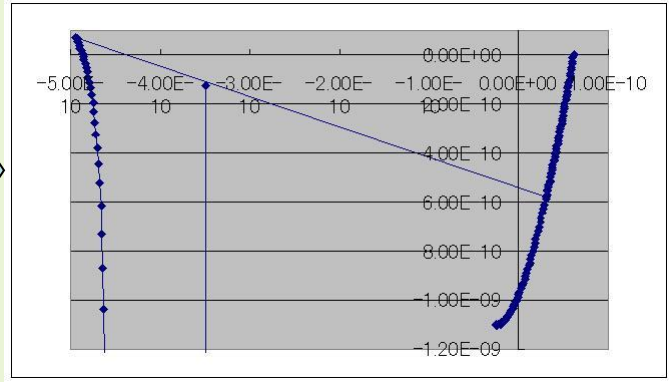
A cantilever is oscillated by an external force with a constant frequency at a single point on the sample surface. A sequential motion of the tip is calculated; the tip contacts to a sample, pushes a sample, and detaches from a sample.





Simulation of the time evolution of the displacement of the tip and the interaction force between the tip and the sample, when the tip contacts to a sample, pushes a sample, and detaches from a sample; in case of a small spring constant.





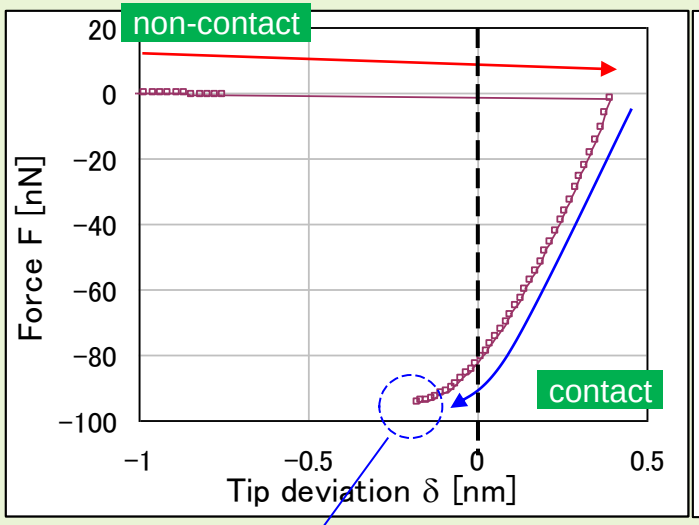
Simulation of the time evolution of the displacement of the tip and the interaction force between the tip and the sample, when the tip contacts to a sample, pushes a sample, and detaches from a sample; in case of a large spring constant.

A Method for Investigating Viscoelastic Contact Analysis

LiqAFM A Method for Investigating Viscoelastic Contact

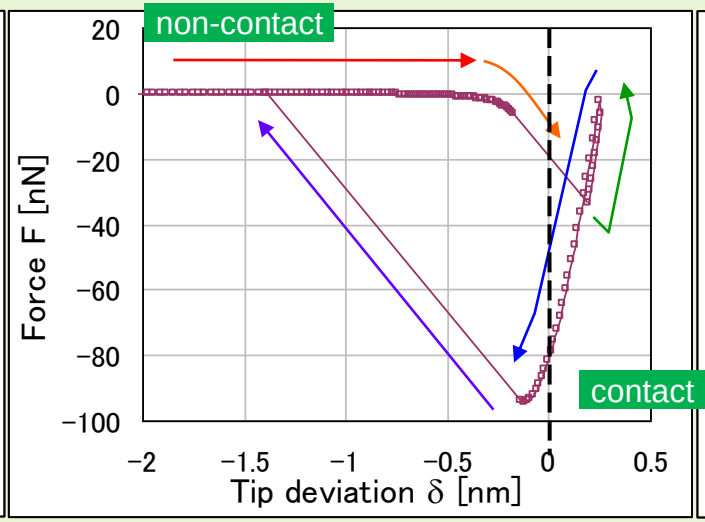
We can simulate a contact between a viscoelastic sample and a tip, and can compute a force curve.

In the case of a cantilever of a small spring constant in vacuum

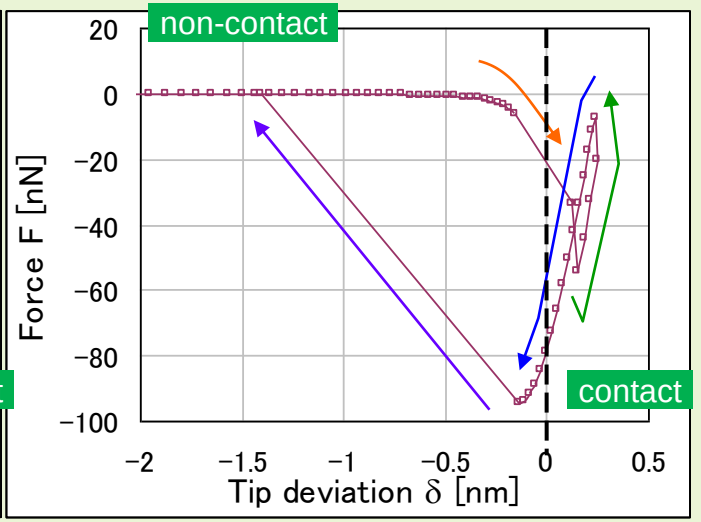


The spring constant is too small that the tip can not overcome adhesion and can not leave the sample.

In the case of a cantilever of a large spring constant in vacuum



In the case of a cantilever of a large spring constant in liquid

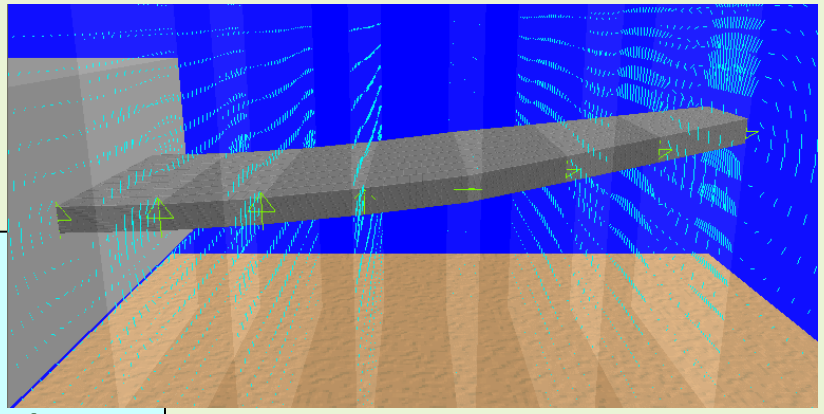


1. The tip moves downwards.
2. The tip becomes in contact with the sample above the surface, and it sinks into the sample.
3. The tip sinks into the sample deepest and the adhesion force become equal to zero.
4. The tip moves upwards.
5. The tip leaves the sample surface.

It is observed that motion of the tip is influenced by fluid in the process of contact between the tip and the sample.

Theory and simulation of dynamic AFM in liquid

LiqAFM



Problem of AFM Theory

Nonlinear effect
Multimode
vibrational
excitation

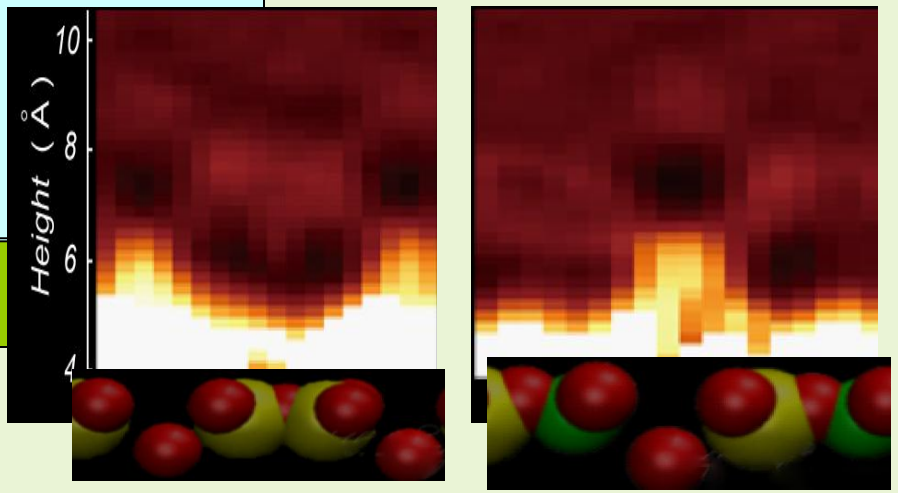
Cantilever oscillation in liquid

Adhesive force
Electric double-
layer

The force affected by
liquid molecules
The structuring of
water

Soft material
Effect of the
viscoelastic
response

AFM image of water on mica
It shows the structuring of water.

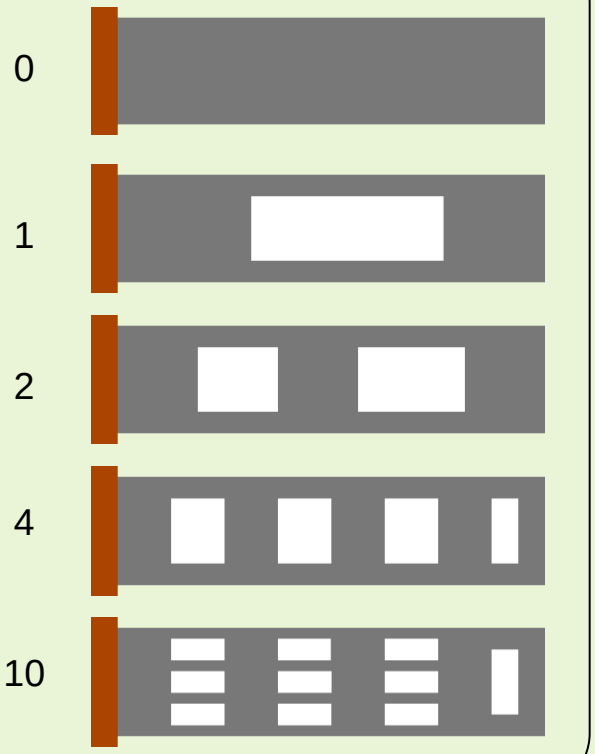


A characteristic oscillation analysis of a cantilever in liquid

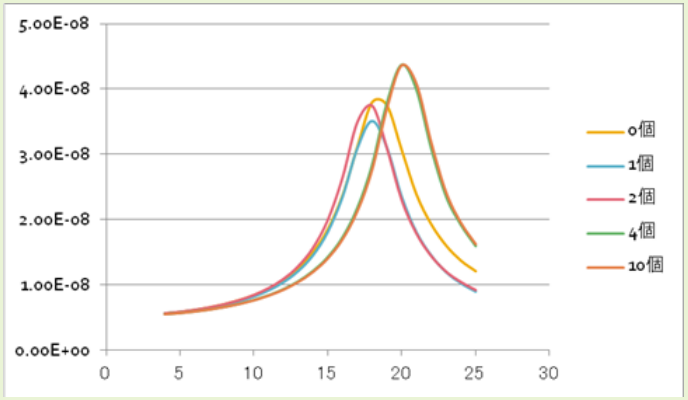
LiqAFM

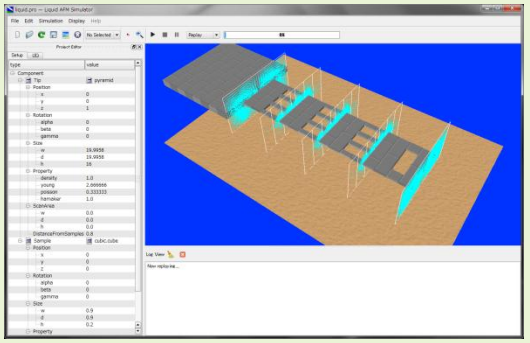
Oscillation of a tabular cantilever in liquid

Making holds on a cantilever



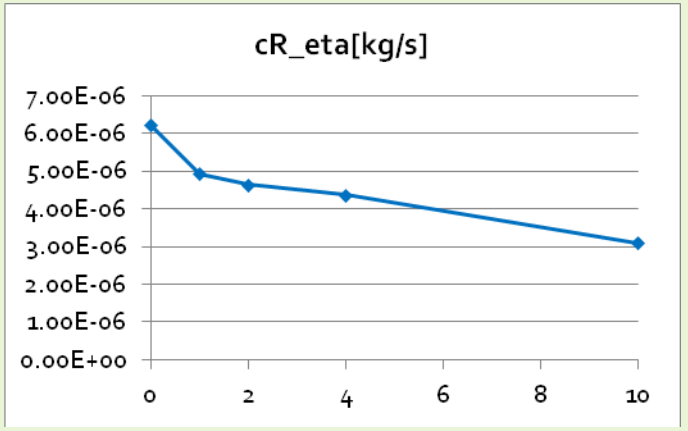
The cantilever is vibrated in liquid. The convergence value of cantilever's amplitude with respect to frequency of forced vibration of the cantilever is calculated.





GUI on which the vibration of a cantilever is simulated.

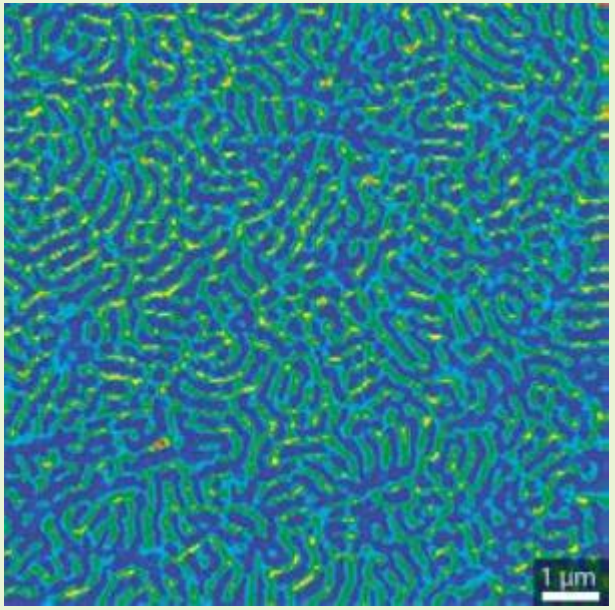
The coefficient of viscous resistance force is gained.



It is understood that the coefficient of viscous resistance force decreases as holes increase.

The prospect to soft material based materials

- In the field of nanobio connection, experiment analysis by the AFM is a tendency to increase.
- The AFM experiments image of biological material such as DNA is measured chronologically.
- The viscoelastic of polymer is measured by AFM measurement.
- Etc.



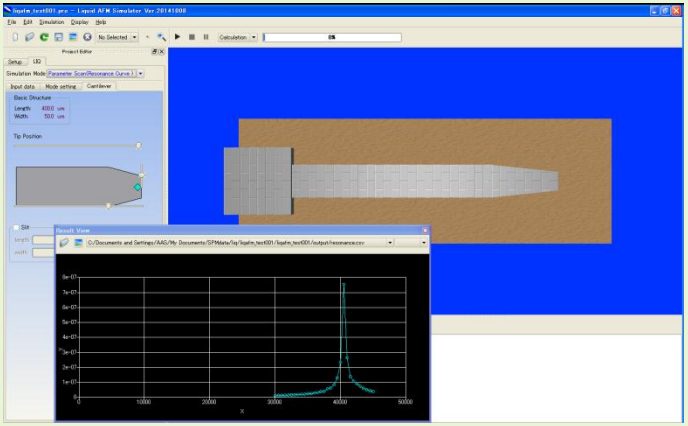
The polymer thin film is observed by AFM,
And its viscoelastic is visualized.
D. Wang et al., Macromolecules 44, 8693–8697 (2011).

The development of our simulator which has a function of the viscoelastic contact analysis become able to simulate such examples.

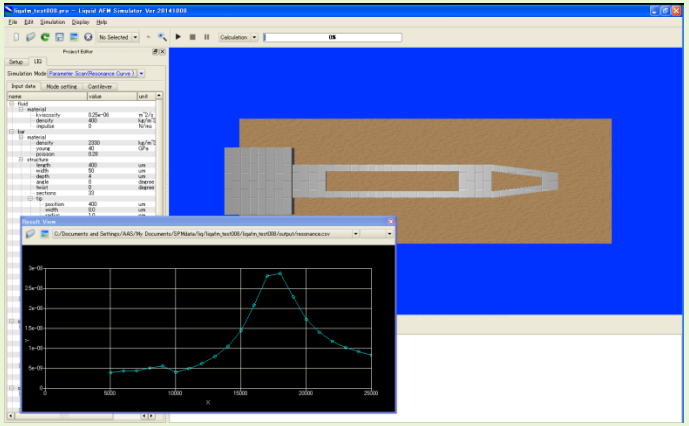
Parameter scan mode

LiqAFM

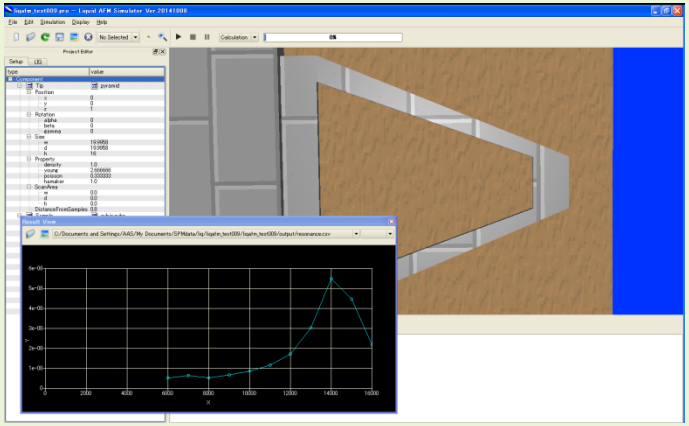
We examine the resonance frequency of the cantilever. At first, we calculate the time evolution of the cantilever motion for a sequence of frequencies, and obtain saturated amplitudes for their frequencies. We then estimate a resonance frequency from a frequency spectrum which is the amplitude of the cantilever vs. the frequency.



We obtain a resonance frequency by simulating a frequency spectrum of a cantilever. **In case of a rectangular cantilver with a single hole in vacuum.**



We obtain a resonance frequency by simulating a frequency spectrum of a cantilever. **In case of a rectangular cantilver with two holes in liquid.**

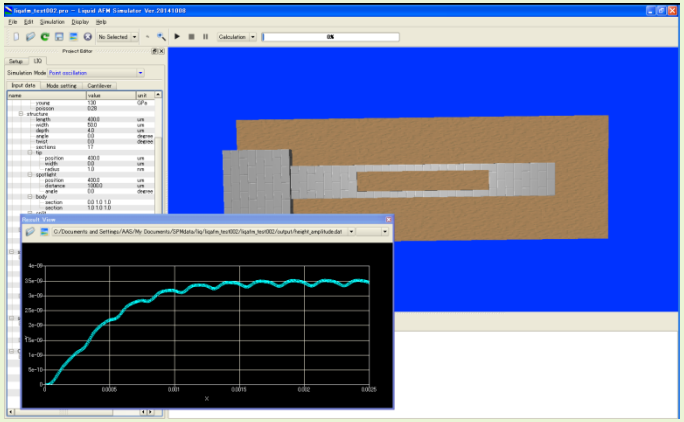


We obtain a resonance frequency by simulating a frequency spectrum of a cantilever. **In case of a triangle cantilver with no hole in liquid.**

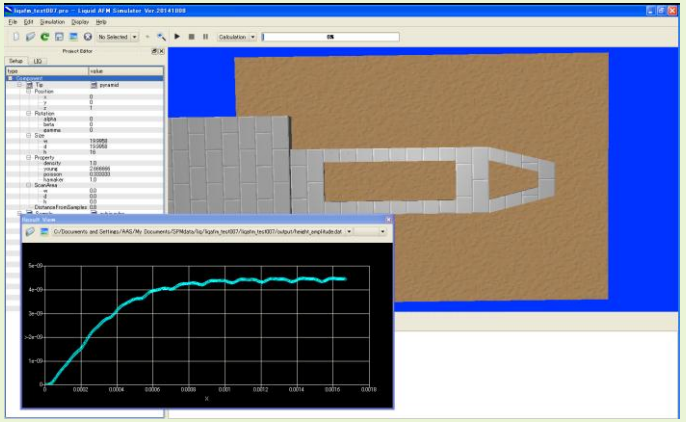
Non-viscoelastic dynamics mode

LiqAFM

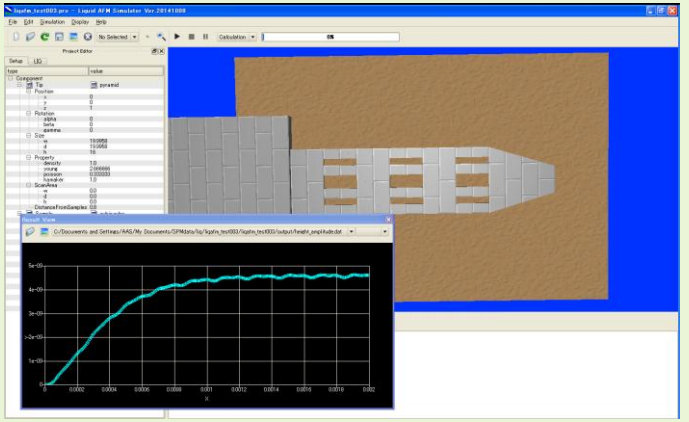
A cantilever is oscillated by an external force with a constant frequency at a single point on the sample surface. A sequential motion of the tip is calculated provided that there is no viscoelasticity of the sample.



•While the external force oscillates the cantilever's tail in liquid, we examine the time evolution of the amplitude of the cantilever's head. The tip is quite far from the sample surface so that the tip does not contact to the sample. **In case of a rectangular cantilver with a single hole.**



•While the external force oscillates the cantilever's tail in liquid, we examine the time evolution of the amplitude of the cantilever's head. The tip is quite far from the sample surface so that the tip does not contact to the sample. **In case of a rectangular cantilver with two holes.**

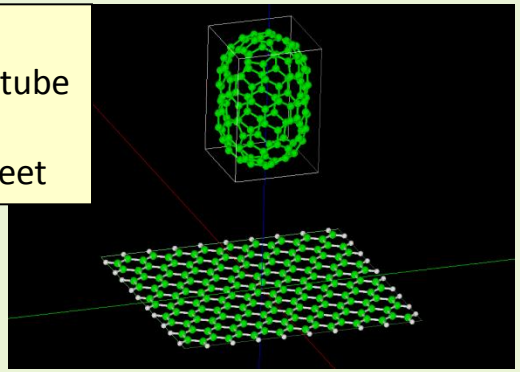


•While the external force oscillates the cantilever's tail in liquid, we examine the time evolution of the amplitude of the cantilever's head. The tip is quite far from the sample surface so that the tip does not contact to the sample. **In case of a rectangular cantilver with a lot of holes.**

The energy curve and the force curve of the system in vacuum / liquid

CG CG-RISM

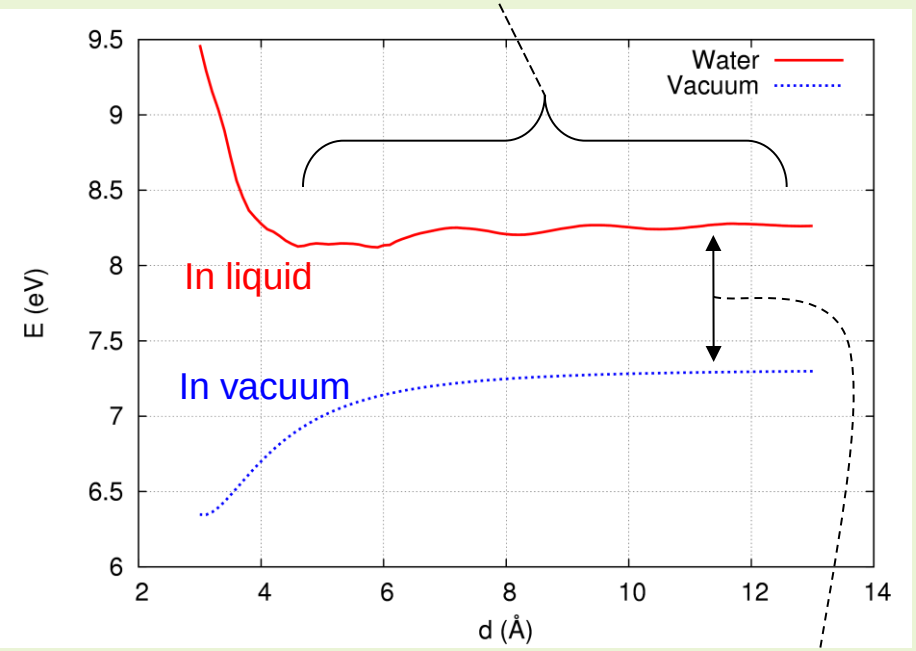
The tip :
Carbon nanotube
The sample:
Graphene sheet



Energy of a system

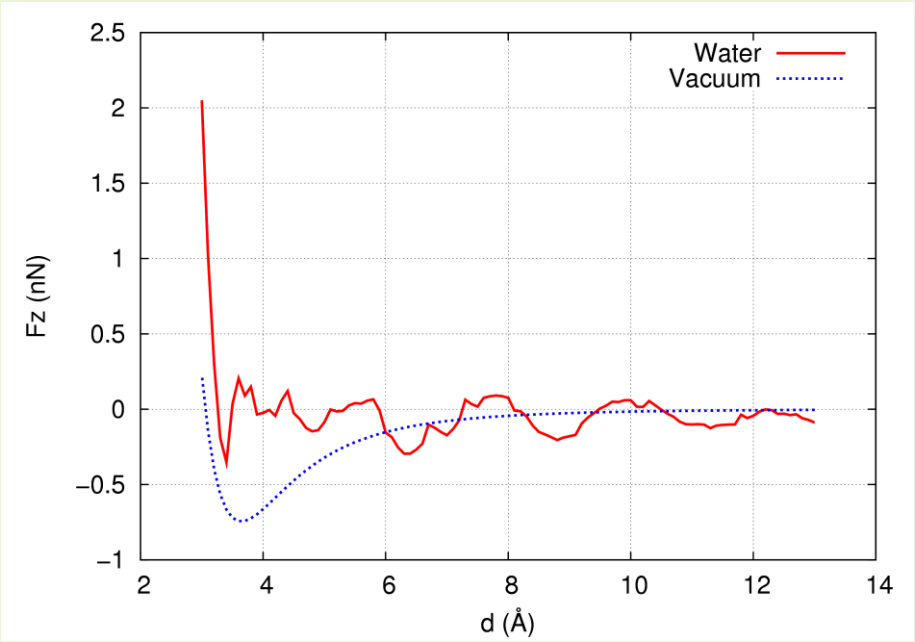
The distance d between the tip and the sample is varied, and the energy of a system is calculated.

Vibration behavior by the hydration structure



Offset by the underwater environment

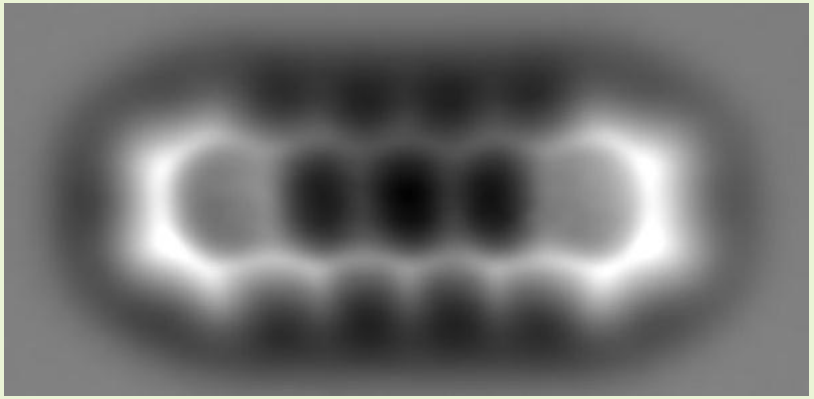
Force curve



(The case of the under the aquatic environment (red line) is a simple numerical differentiation.)

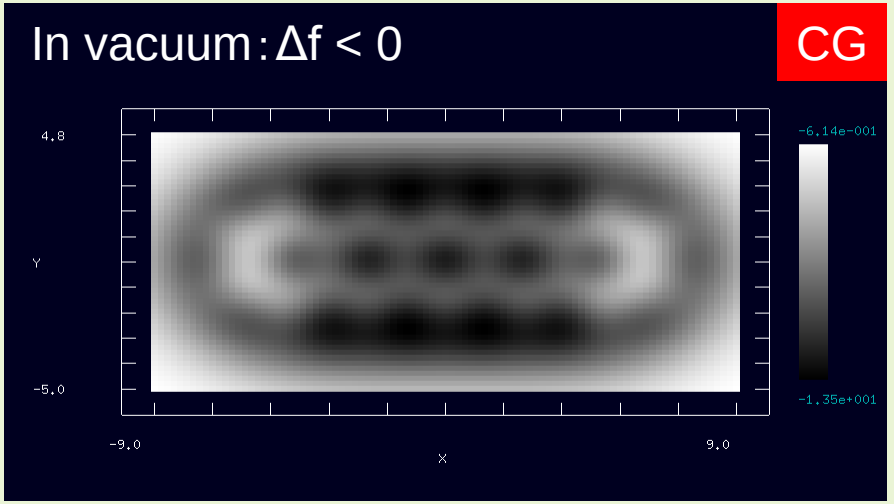
Observation and simulation of AFM frequency shift image of pentacene

The observation of the frequency shift image



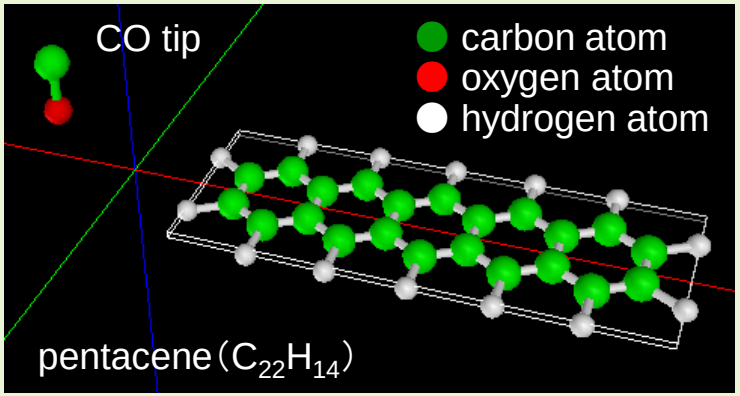
L. Gross *et al.*, Science **325**, 1110-1114 (2009).

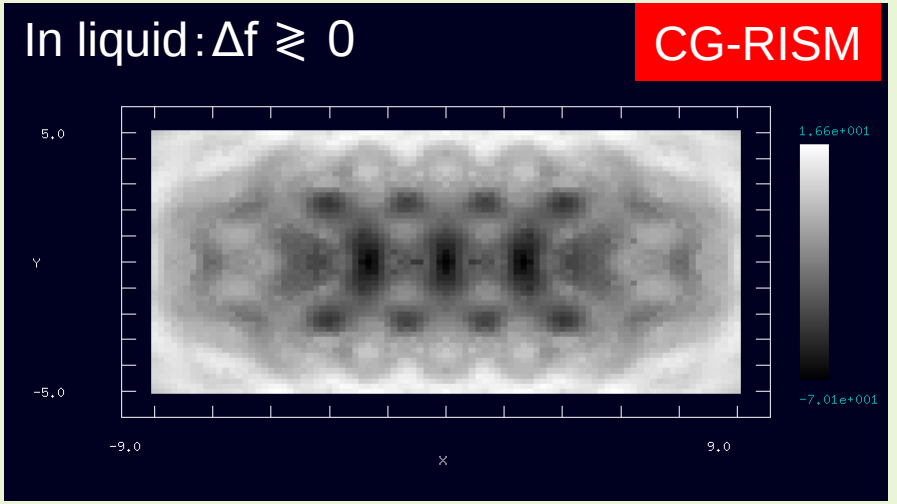
The simulation of the frequency shift image



Good agreement

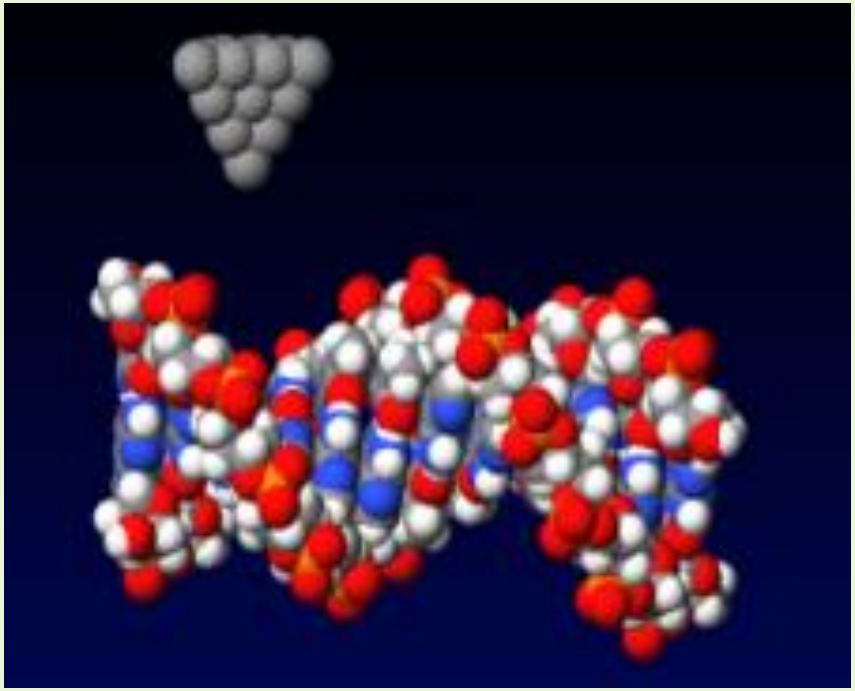
It can also simulate in the case of in water.



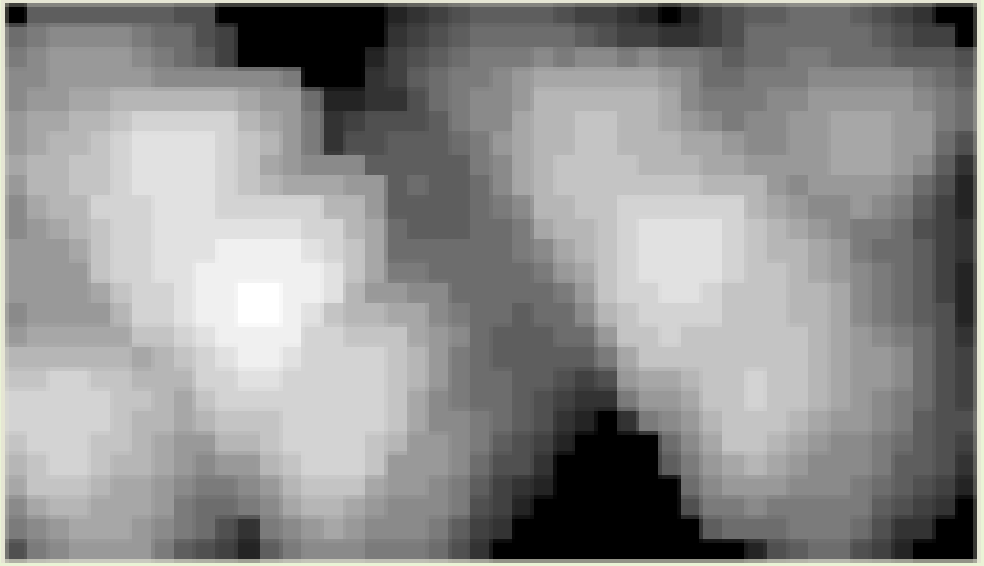


Example of NC-AFM topography image

DNA model

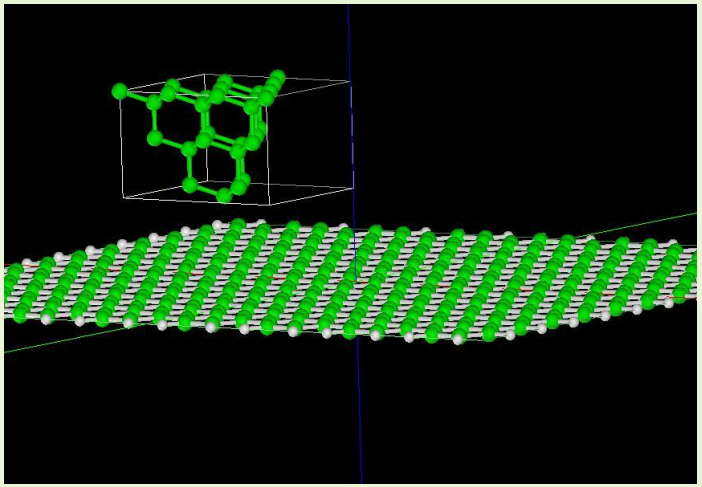


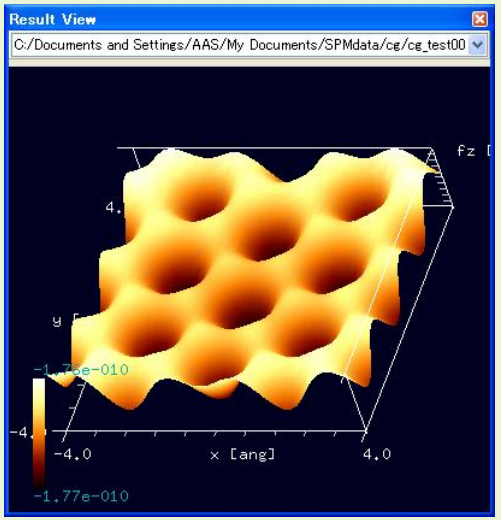
Simulation result



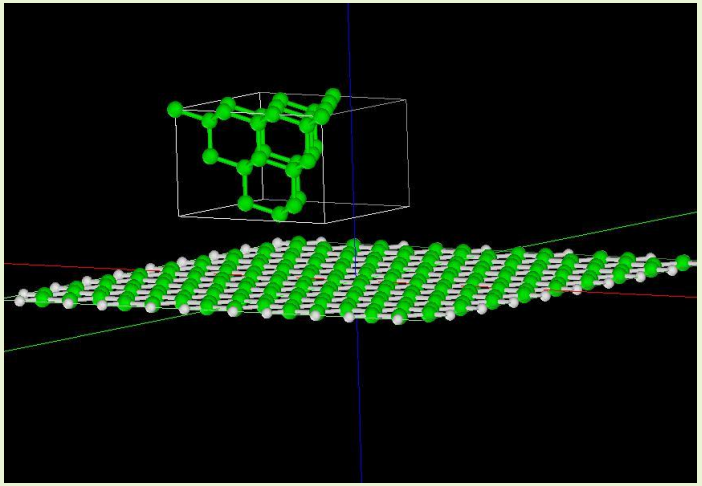
Constant-height mode

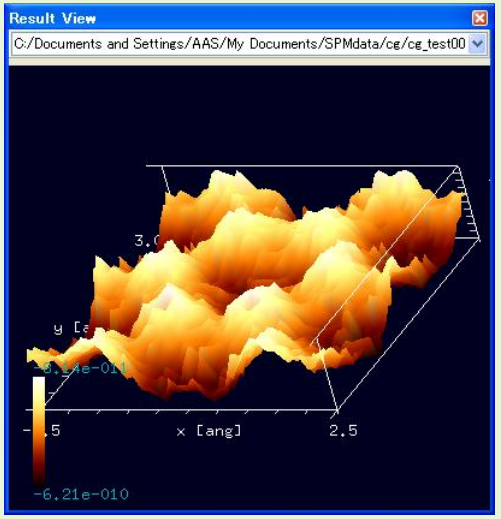
CG CG-RISM We derive the forces to the tip which scans on the sample surface at a constant height.





•The AFM simulation of a graphene sheet by a diamond tip in the constant-height mode; **in vacuum.**



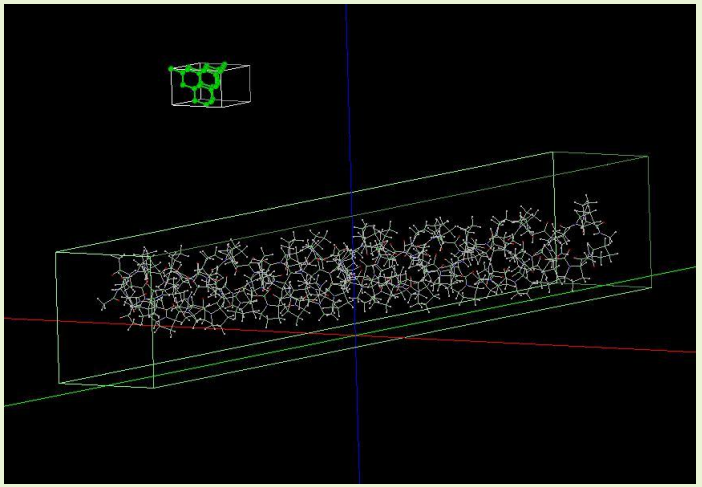


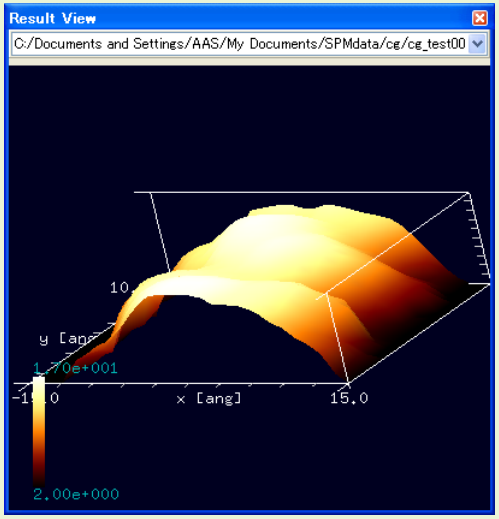
•The AFM simulation of a graphene sheet by a diamond tip in the constant-height mode; **in water.**

Constant-force mode

CG

We search the tip heights on the sample surface where the force to the tip is equal to the specified value. (Not available for a calculation in water)



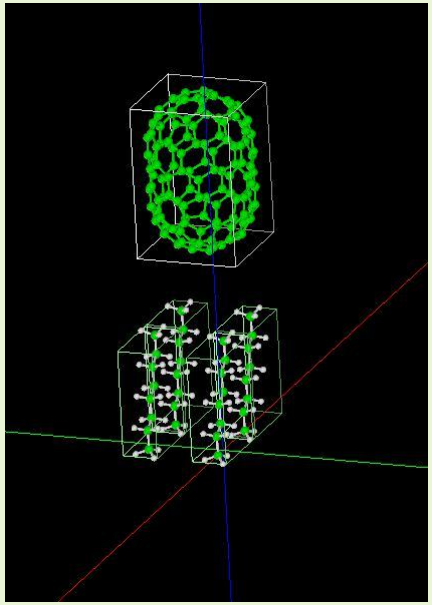


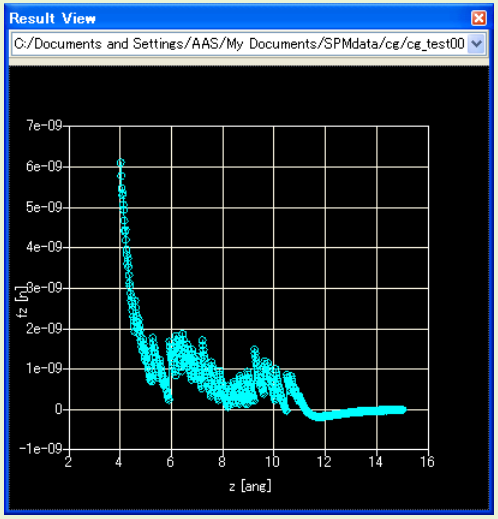
•The simulation of a collagen by a diamond tip in the constant-force mode in vacuum.

Force curve measurement mode

CG CG-RISM

We derive the forces to the tip which comes up to the sample at a specified position on the sample surface.



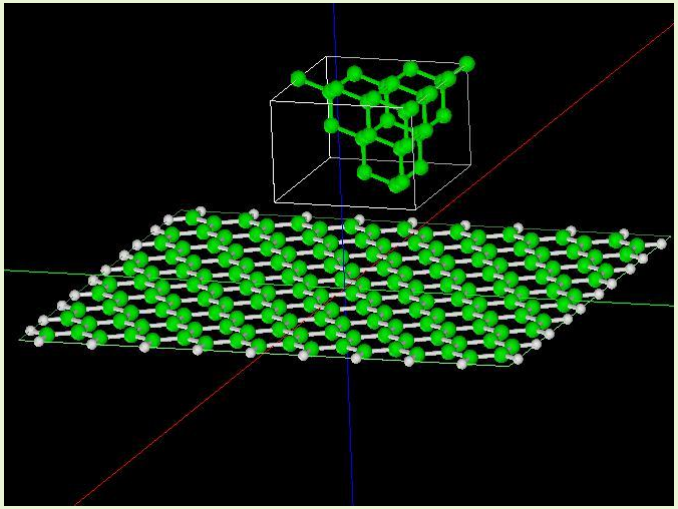


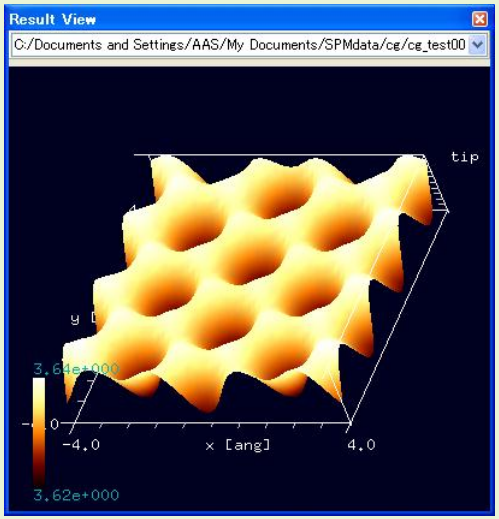
•The force curve simulation of a set of four octance chains by a carbon nanotube tip in the force curve measurement mode in vacuum, considering that the deformation of the atomic configuration in the sample molecules.

Minimum power mode

CG

We search the tip heights on the sample surface where the force to the tip may be minimum. (Not available for a calculation in water)





•The simulation of a graphene sheet by a diamond tip in the minimum power mode in vacuum.

Case study of Classical Force Field AFM Simulator

MD

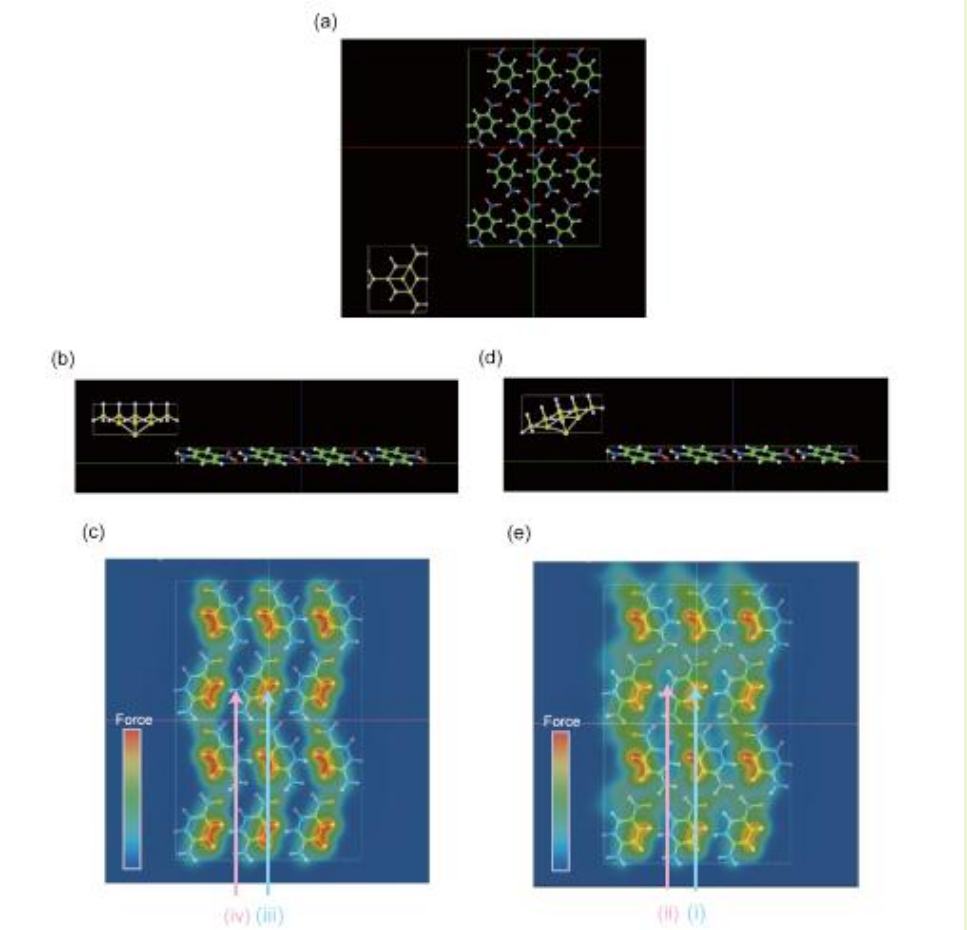


Figure S1. *p*-Nitroaniline (101) surface and Si_{10} tip. Top and side views of the symmetric tip are shown in panels a and b. The simulated tip-surface force distribution is in panel c. The tip was tilted by 17° as shown in panel d and the force simulated with the tilted tip is shown in panel e.

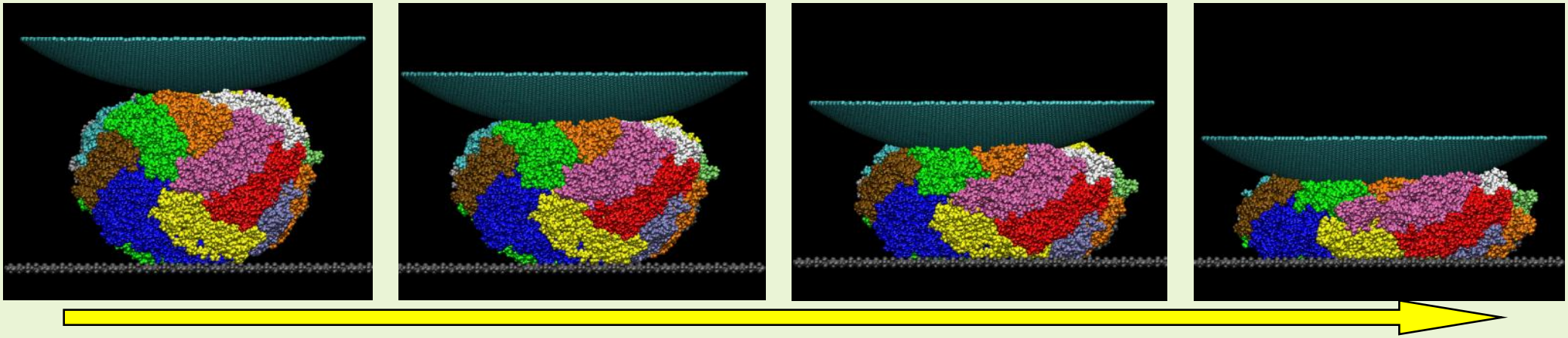
The simulator was utilized in Onishi Laboratory, Department of Chemistry, Kobe University.
（Nishioka et al., J. Phys. Chem. C 117, 2939-2943 (2013).）

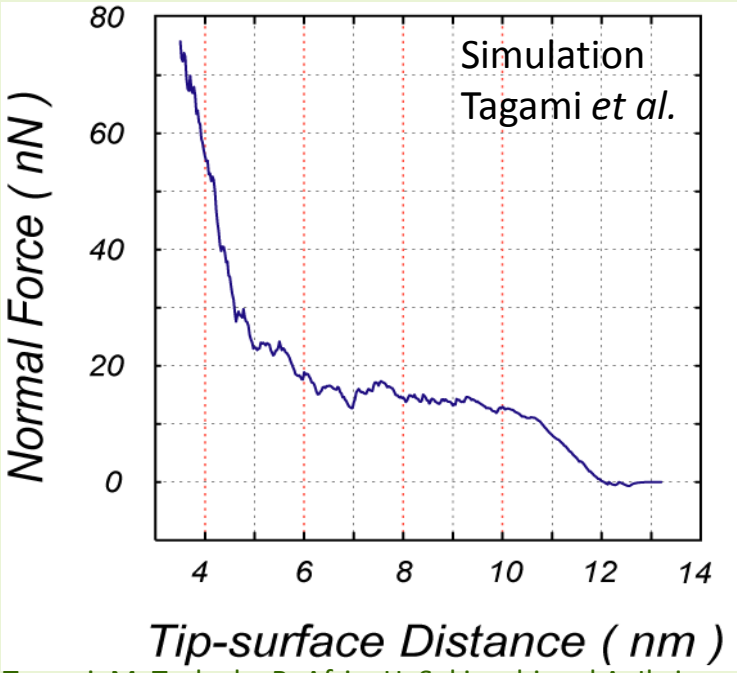
Lower left: the force map of the surface of p-nitroaniline crystal by our "Molecular Dynamics AFM Image Simulator (MD)"
(It appears on Supporting Information of the above thesis.)

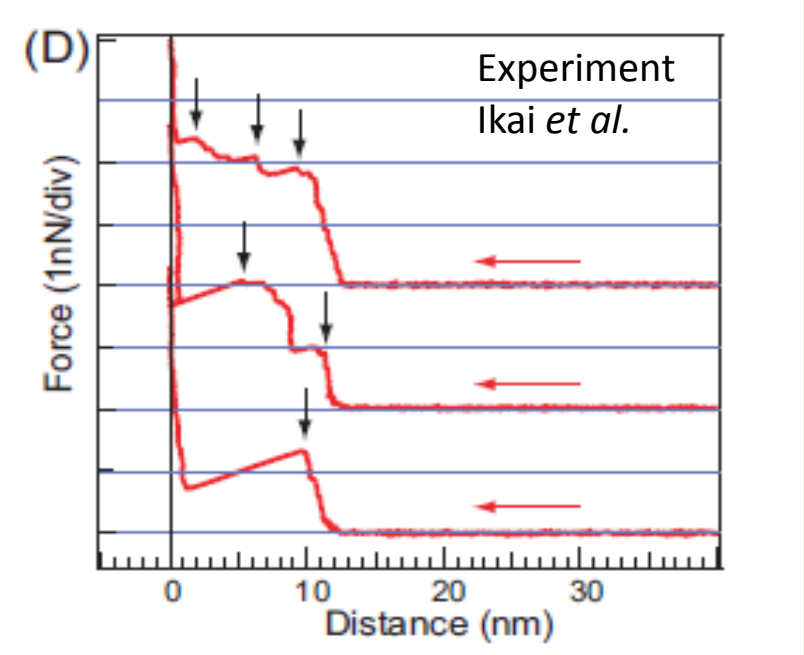
It was used for interpreting of the observed constant frequency shift topography, and it gave a theoretical support on the consideration that the main reason for significantly changing the topography is due to the tilted tip.

Compression simulation of apo-ferritin

MD **Nano-mechanical experiments of protein molecule**







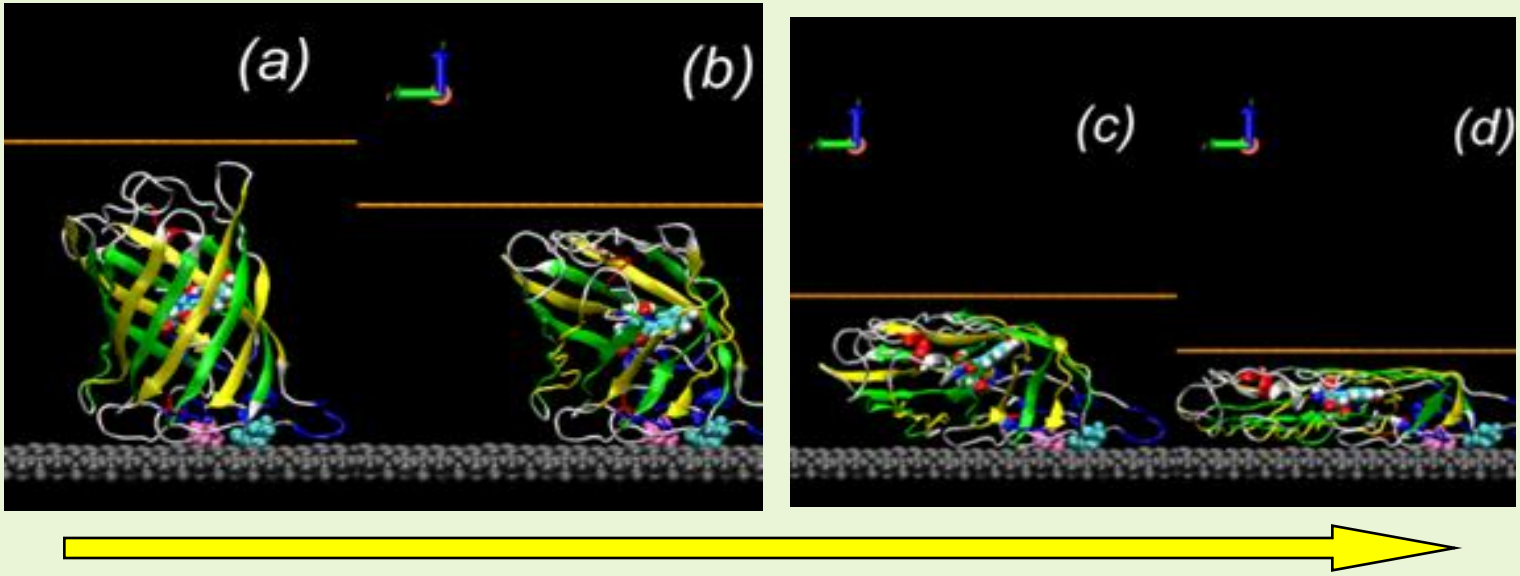
K. Tagami, M. Tsukada, R. Afrin, H. Sekiguchi and A. Ikai,
e-J. Surf. Sci. Nanotech. 4, 552-558 (2006).

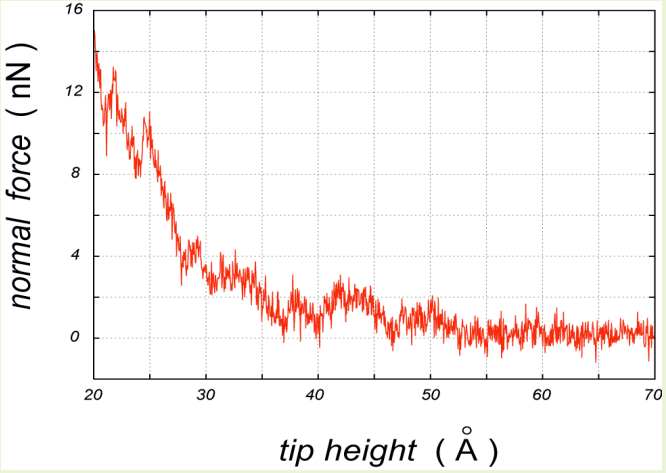
Compression simulation of GFP

MD **Nano-mechanical experiments of protein molcule**

GFP = Green Fluorescent Protein

MD simulation of compression

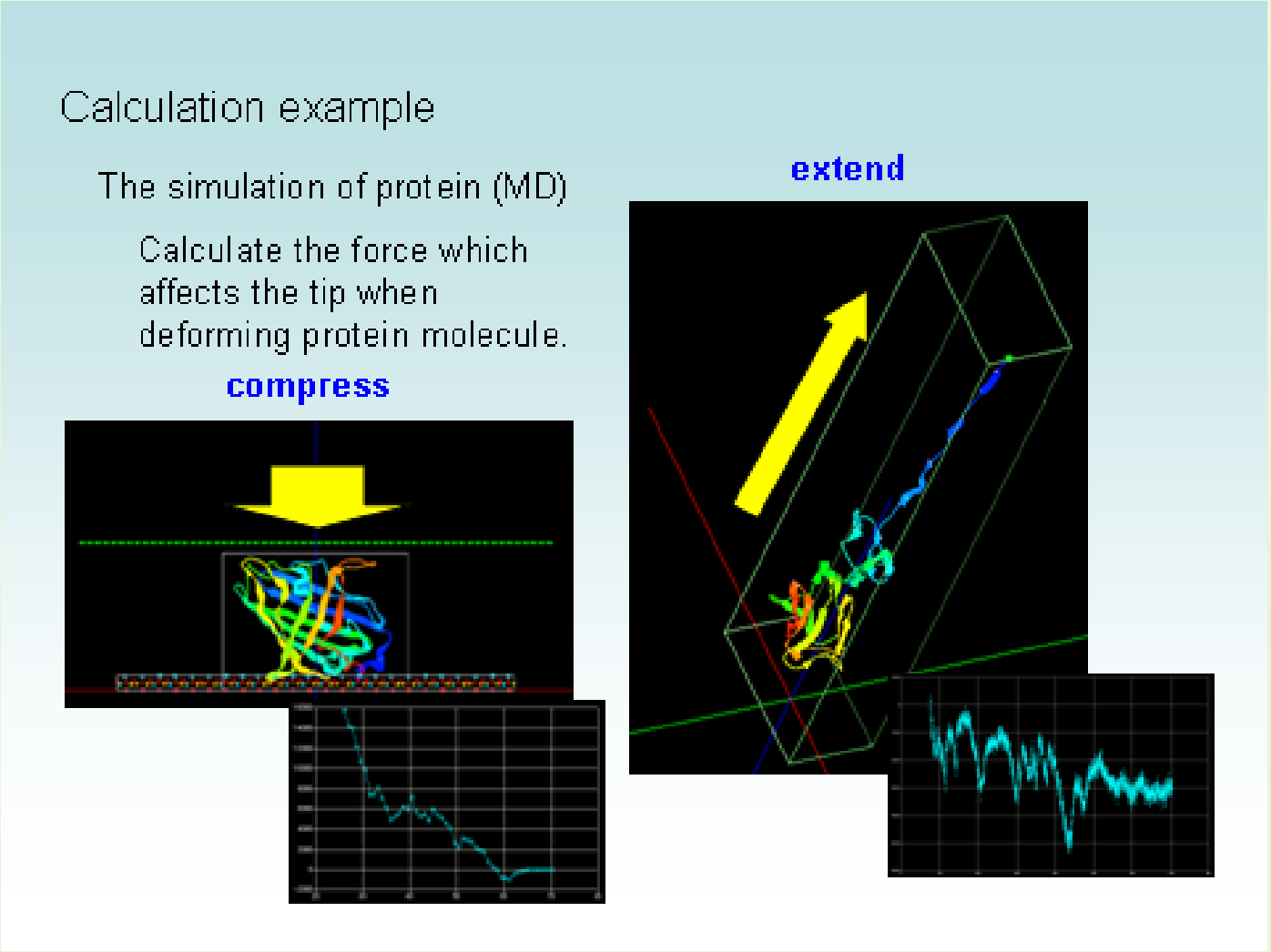




Q. Gao, K. Tagami, M. Fujihira and M. Tsukada, Jpn. J. Appl. Phys., 45, L929 (2006).

Compression and extension experiments of protein molecules by MD

MD **Nano-mechanical experiments of protein molecule**

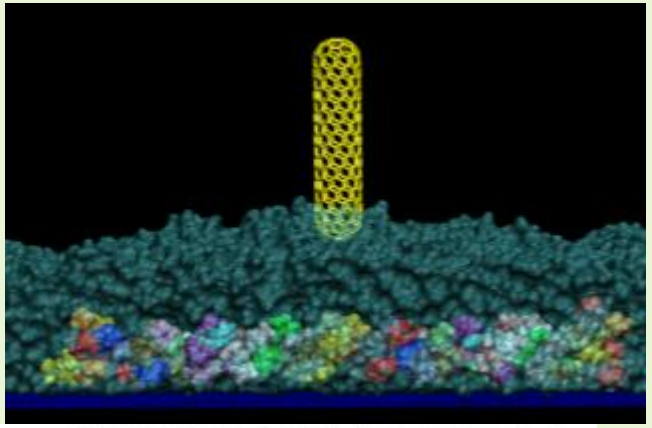


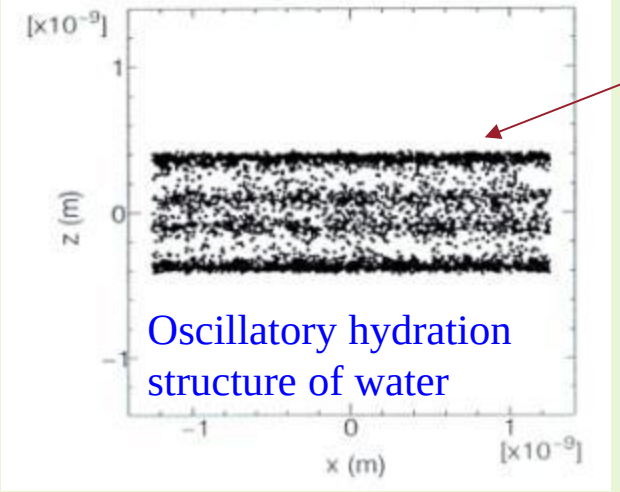
MD can calculate the force curve of simulation which is the compression/extension of protein molecules by the graphite tip.

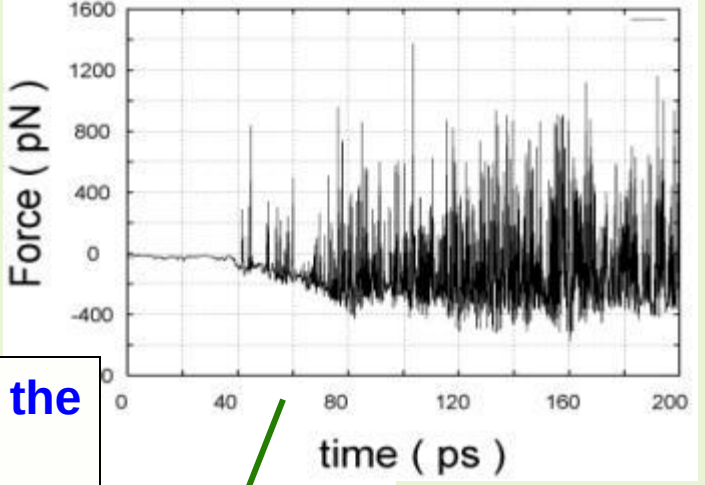
Microscopic structures of water in the vicinity of the object

MD **In the case of Collagen @ graphite**

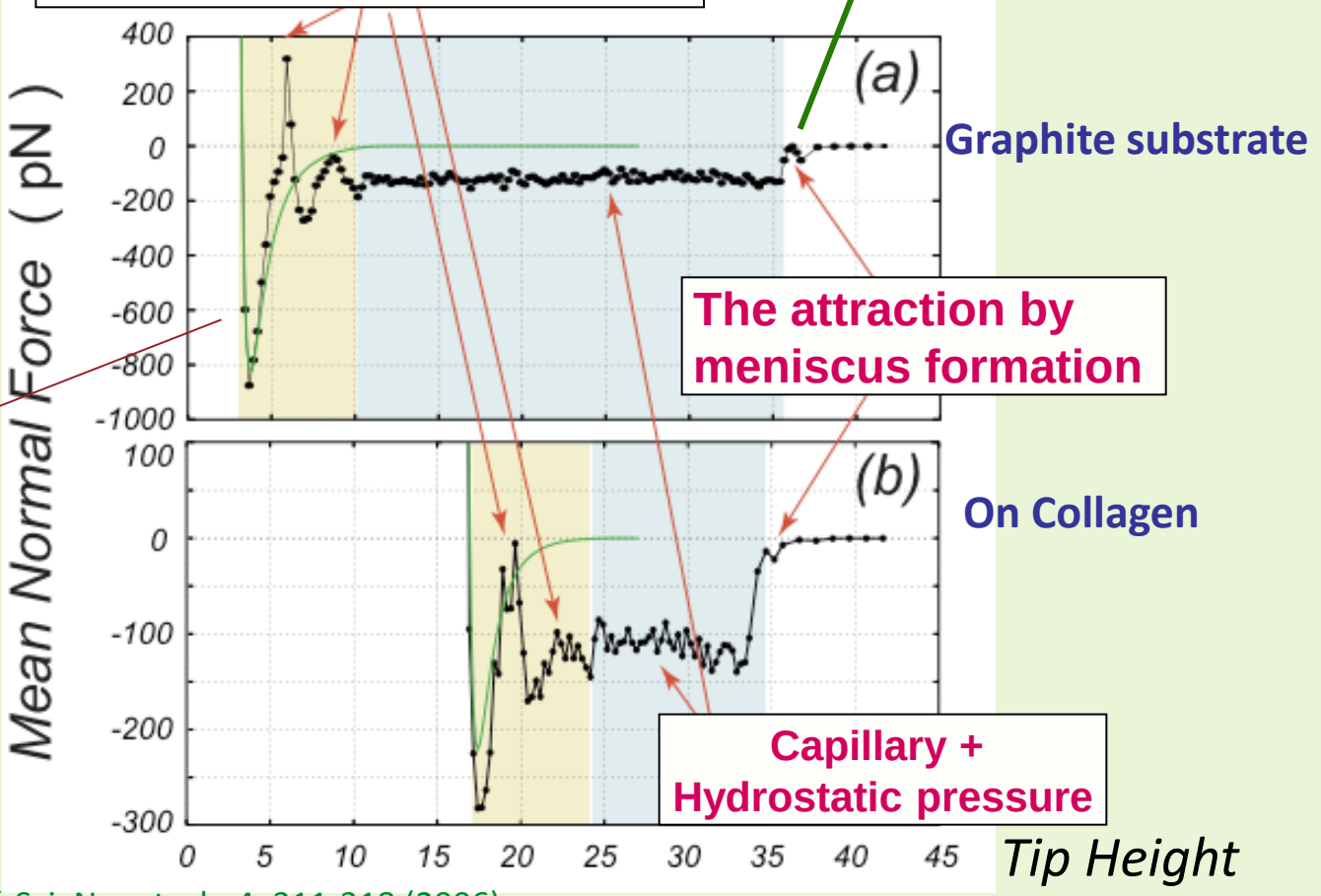
AFM simulation by classical molecular dynamics method (CNT tip)







Oscillatory force reflects the hydration structure



Graphite substrate

The attraction by meniscus formation

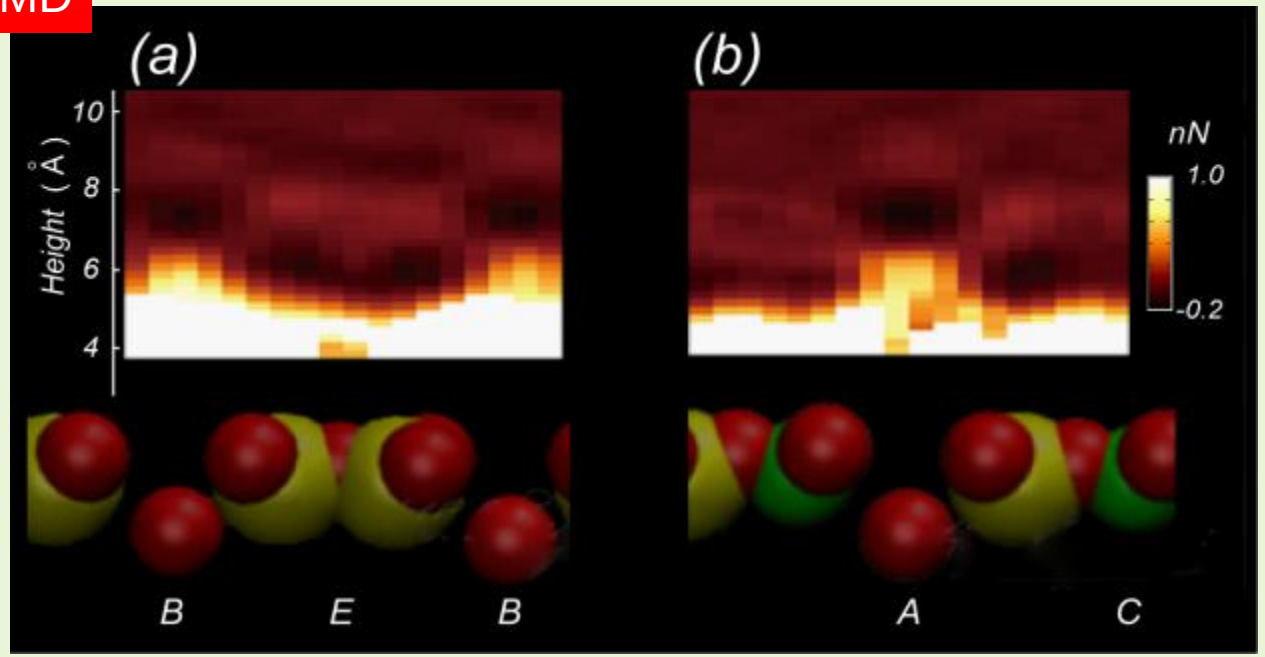
On Collagen

Capillary + Hydrostatic pressure

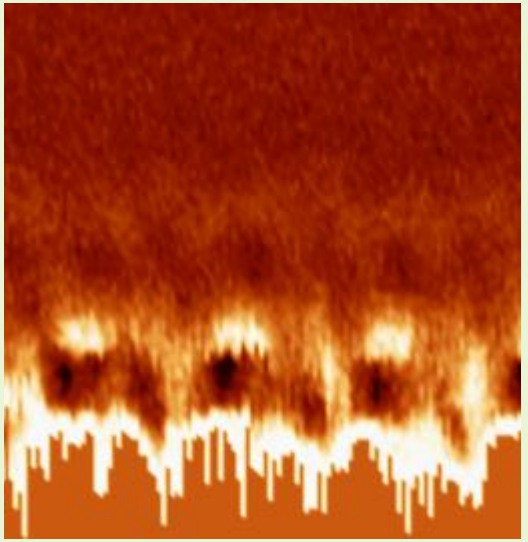
K. Tagami and M. Tsukada, e-J. Surf. Sci. Nanotech. 4, 311-318 (2006).

Interfacial structure of mica surfaces and water

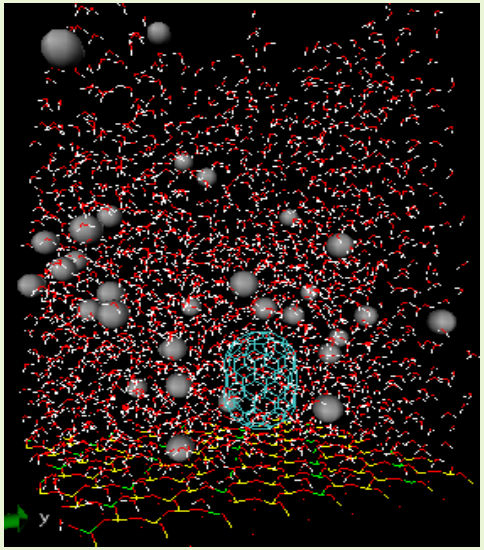
MD **Aspect of force distribution** **Hydration structure is in 3D basis.**



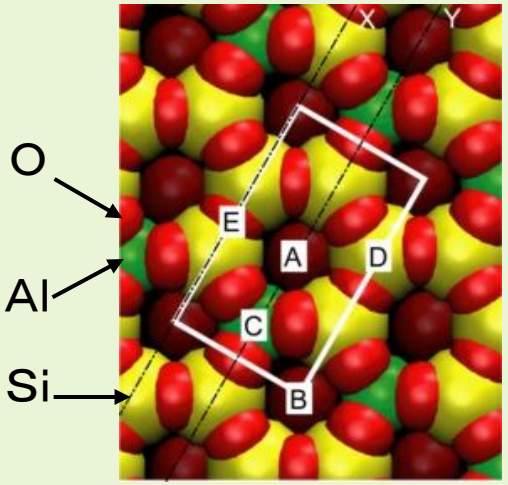
AFM experiment
(The original image is provided by Professor Yamada, Kyoto University.)



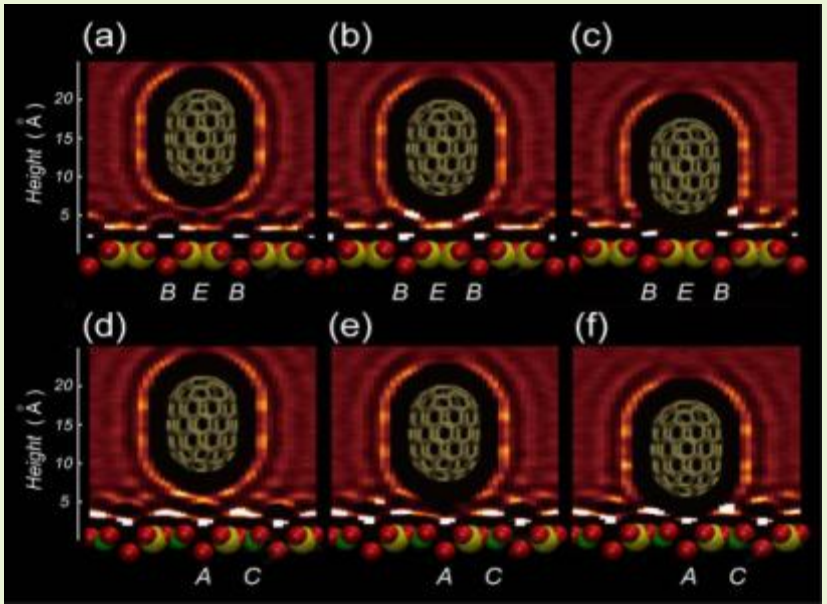
Snapshot in MD



Mica sample model



Distribution of water molecules

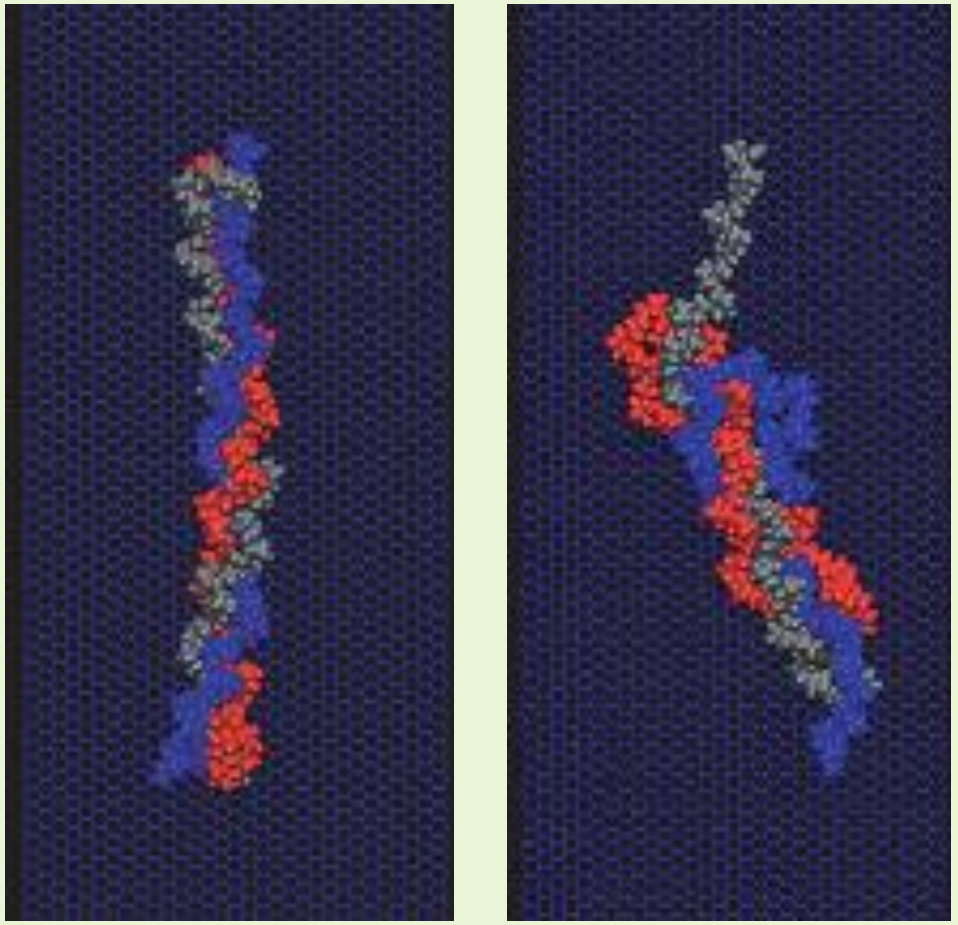


AFM imaging simulation of collagen on the HOPG substrate

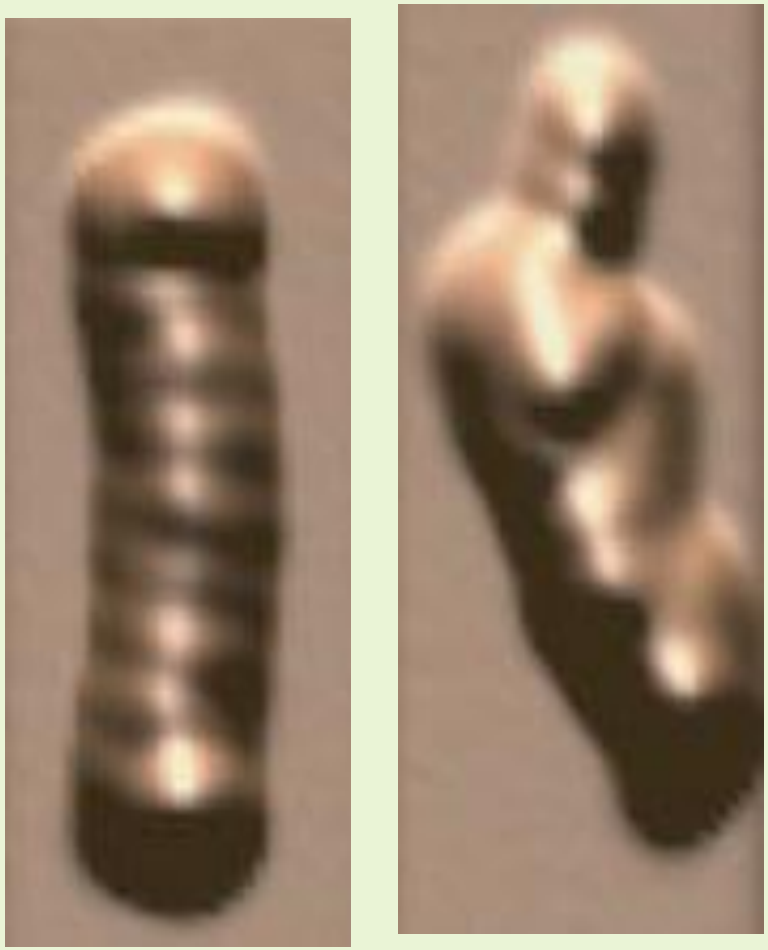
Example of AFM imaging simulation

AFM imaging of collagen adsorbed to the HOPG substrate

Molecular model



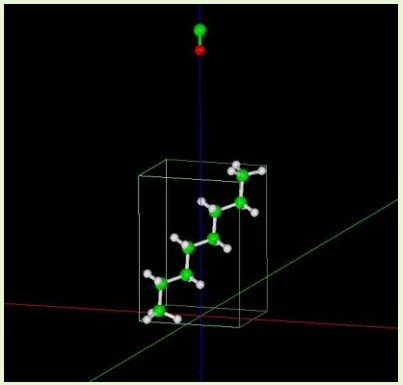
Simulation result

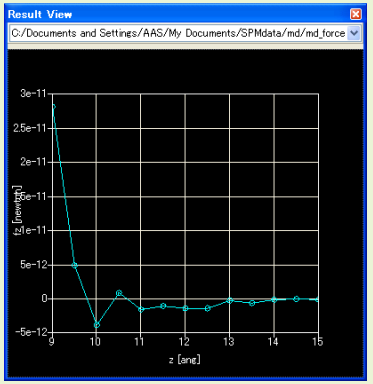


Katsunori Tagami and Masaru Tsukada, e-J. Surf. Sci. Nanotech. Vol. 4 (2006) 294-298.

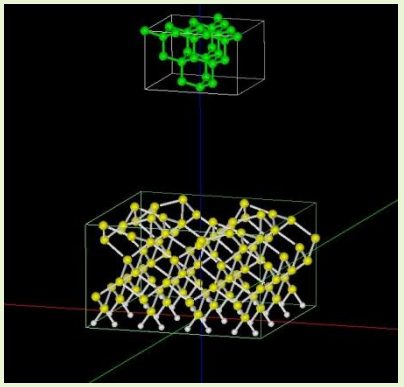
Force curve measurement mode

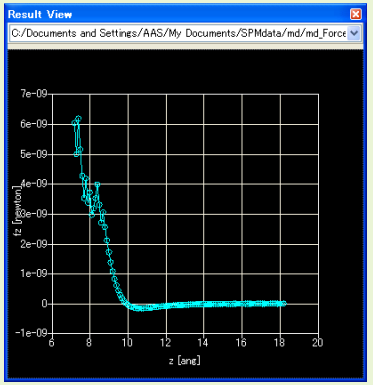
MD We derive the forces to the tip which comes up to the sample at a specified position on the sample surface.



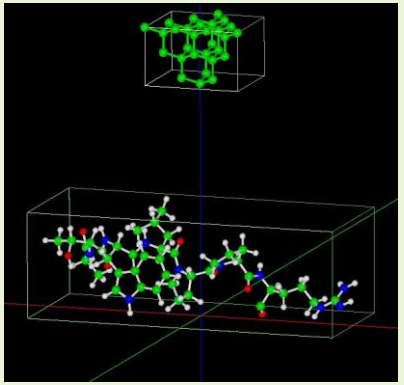


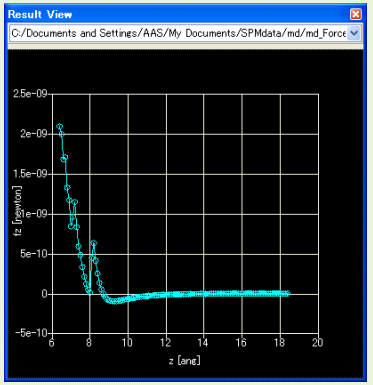
•The force curve of an octane molecule.





•The force curve of a Si(001) surface.

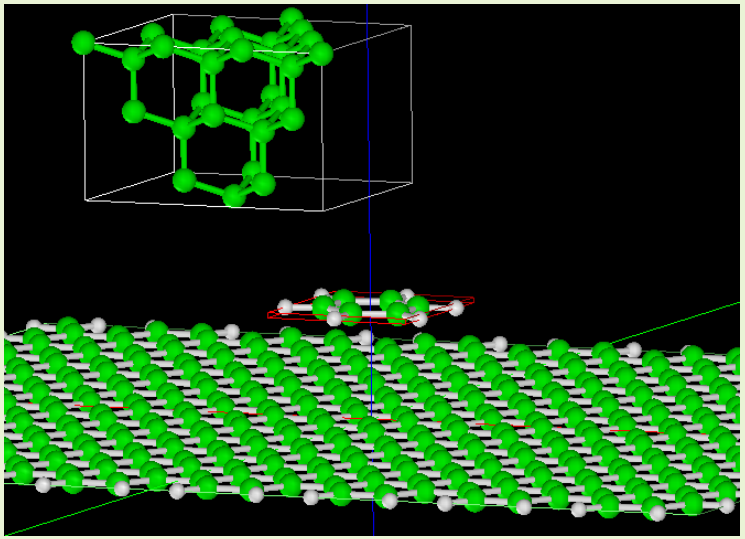


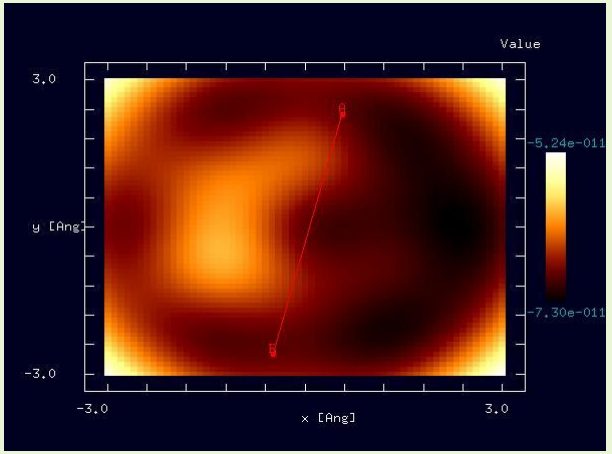


•The force curve of the antiangiogenic ATWLPPR peptide.

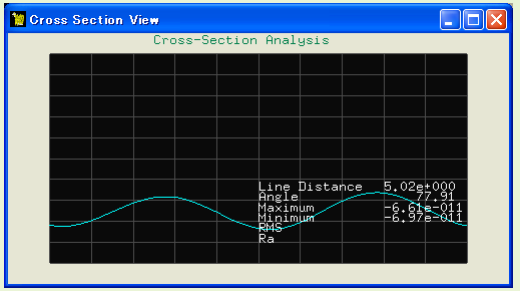
Constant-height mode

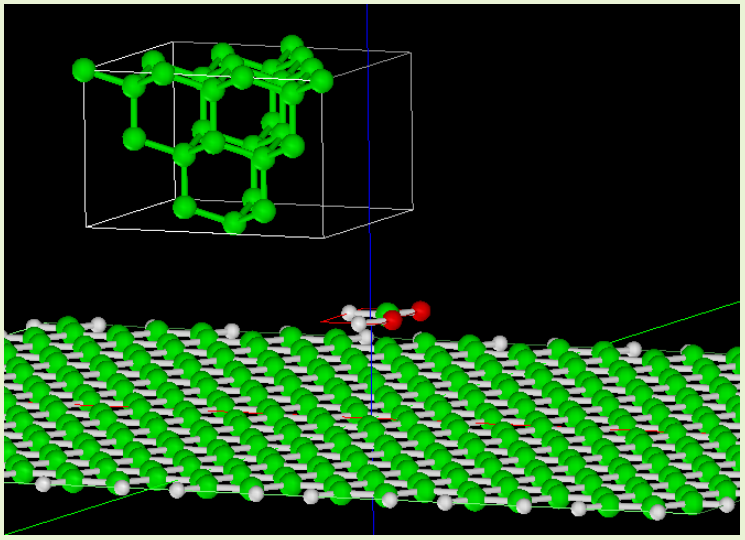
MD We derive the forces to the tip which scans on the sample surface at a constant height.

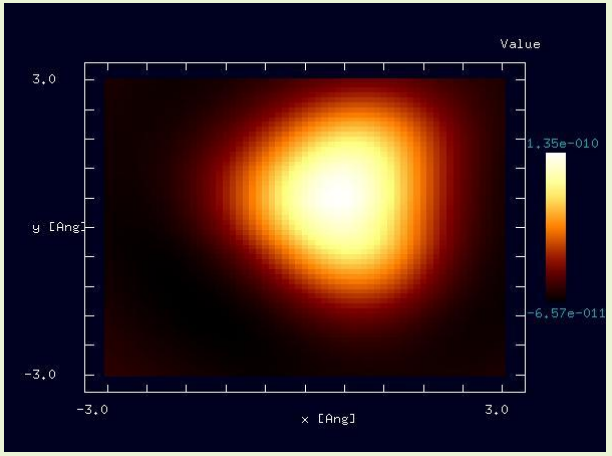




•The simulation of the forces to the tip on a benzene on HOPG in constant-height mode.





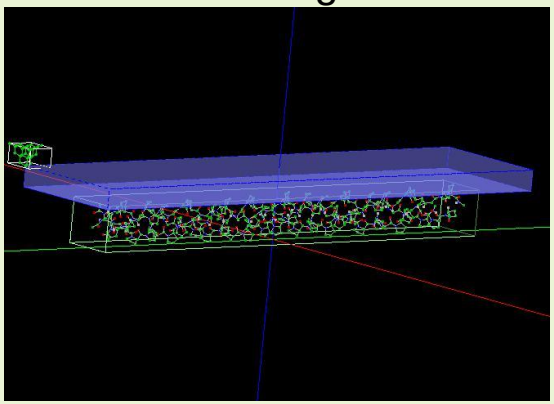


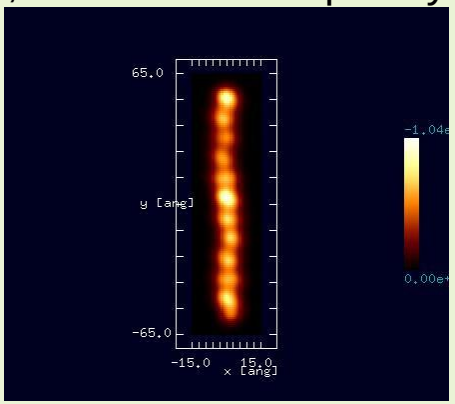
•The simulation of the forces to the tip on a formic acid on HOPG in constant-height mode.

Non-contact mode height constant

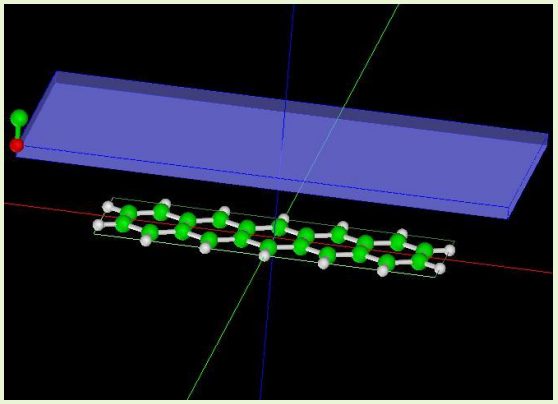
MD

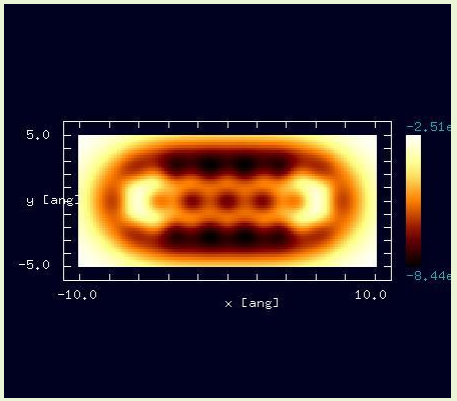
We derive the forces to the tip which scans on the sample surface while oscillating around a constant height. As a result, we obtain a frequency shift image and an energy dissipation image.



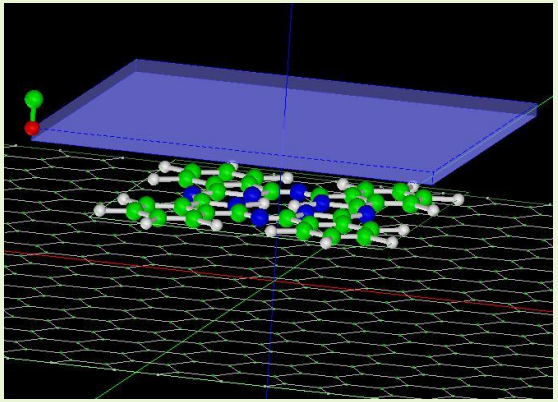


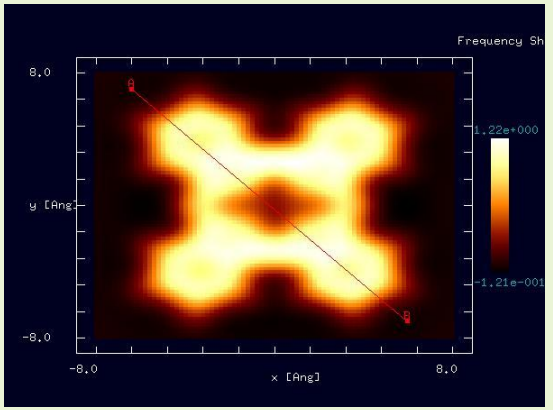
•The simulation of the frequency shift image of a **collagen** in the non-contact mode.



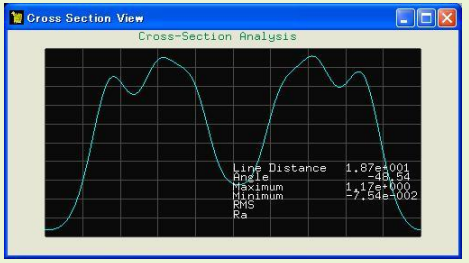


•The simulation of the frequency shift image of a **benzene** in the non-contact mode.





•The simulation of the frequency shift image of a **phthalocyanine** in the non-contact mode.

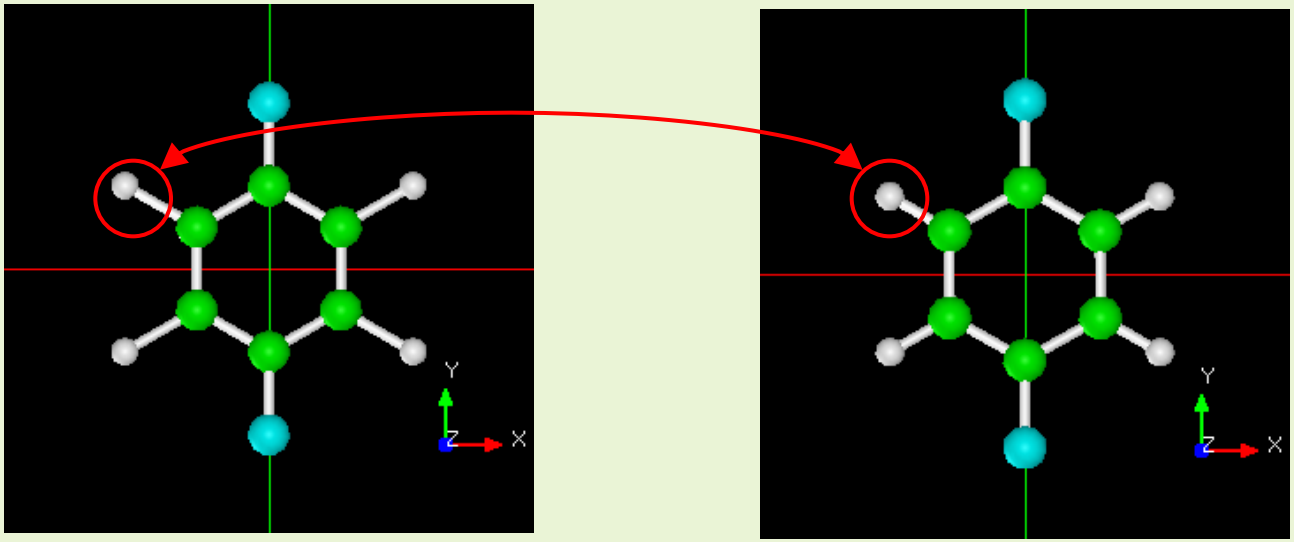


Relaxation

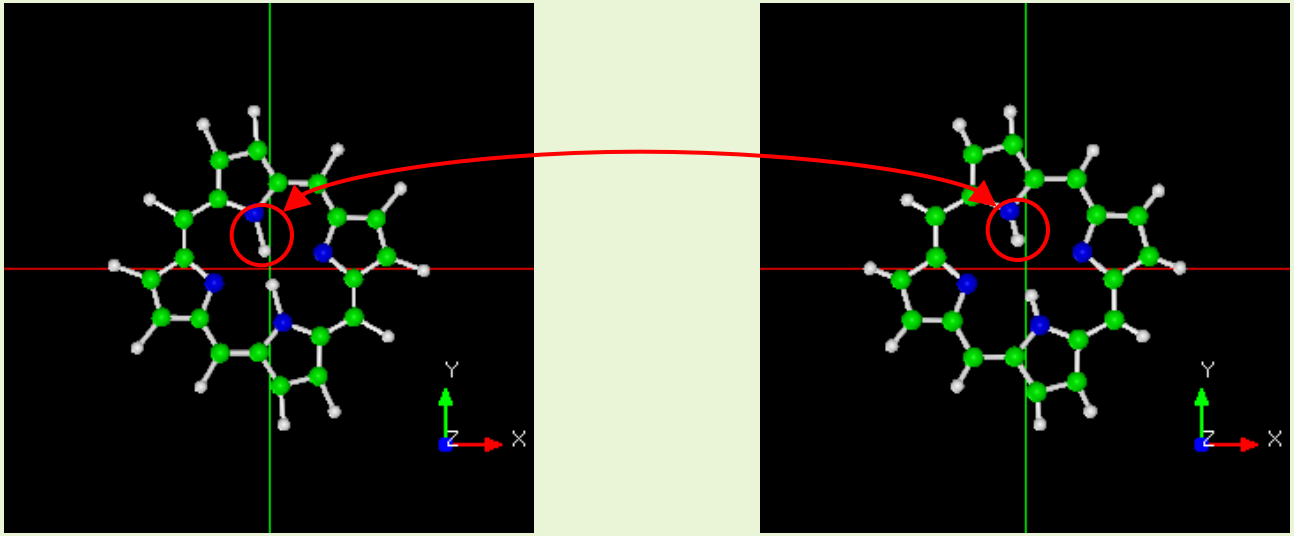
MD We calculate the structural relaxation of a sample molecule as a preparation for a simulation.

Before

After



The structural relaxation of a **dichlorobenzene**

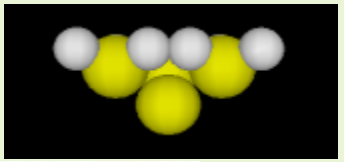


The structural relaxation of a **porphyrin**

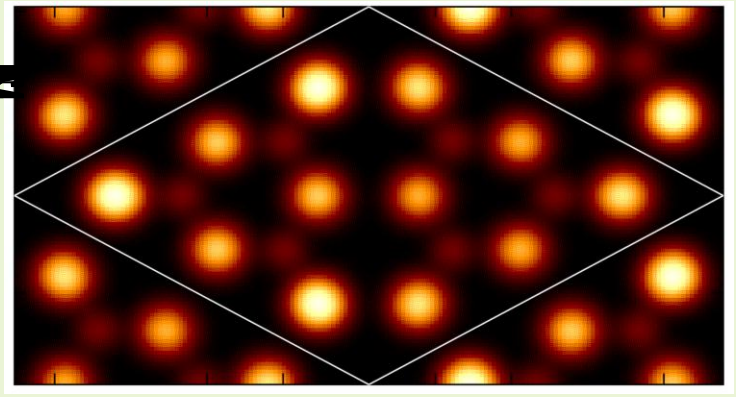
Simulation of STM by Bardeen's perturbation method and DFTB method

-Calculation of the tunneling current-

DFTB **STM simulation**

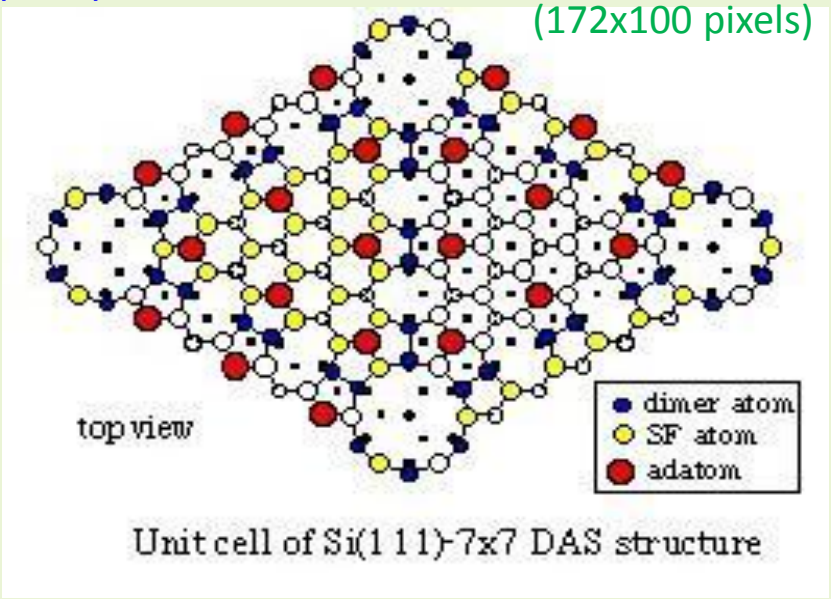


Si_4H_9 tip; tip height = 4.0 Å



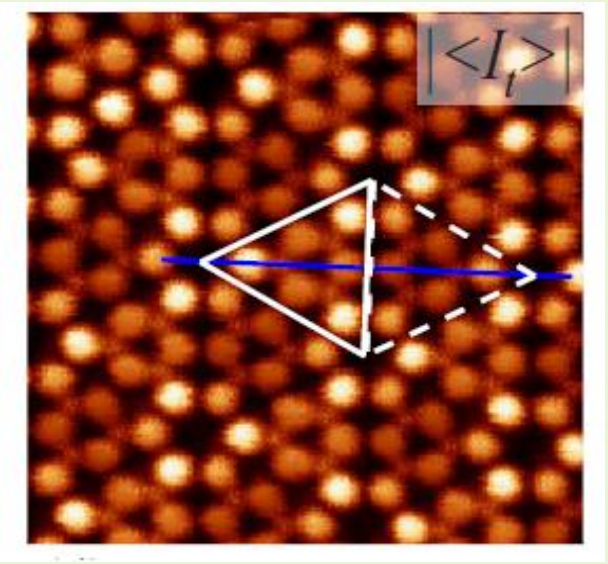
Si(111)-7x7 DAS structure

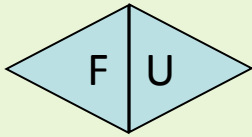
Computation time 1.5 hours
(172x100 pixels)



Unit cell of Si(1 1 1)-7x7 DAS structure

experiment by Sawada et al. (2009)

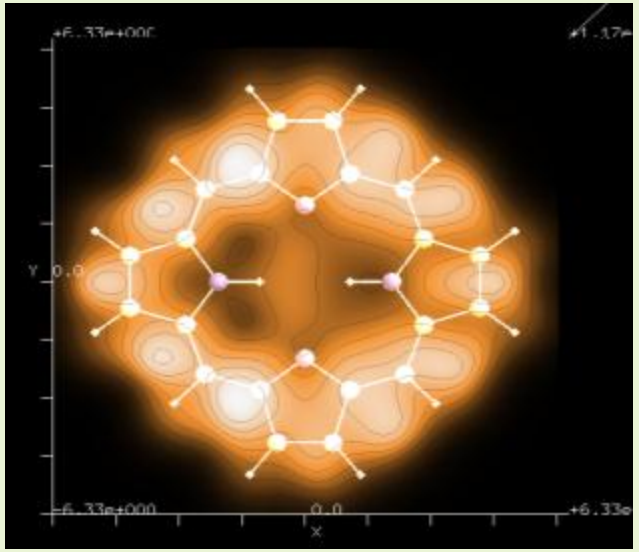


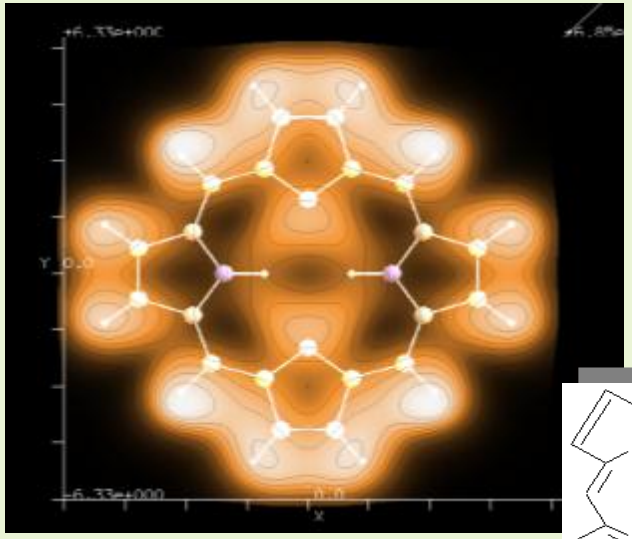


It reproduces the difference in brightness between region F and region U.
It reproduces that looks slightly restatom.

STM image of Porphyrin

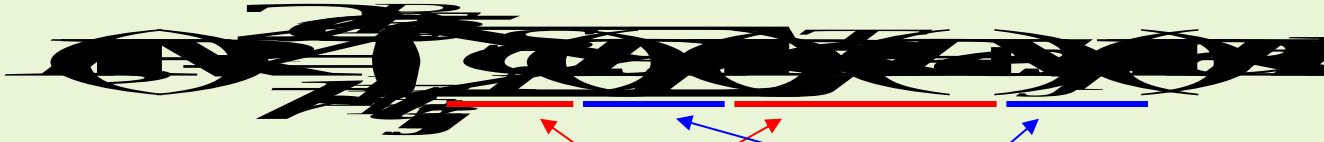
DFTB (W tip : 6s,5d orbitals)





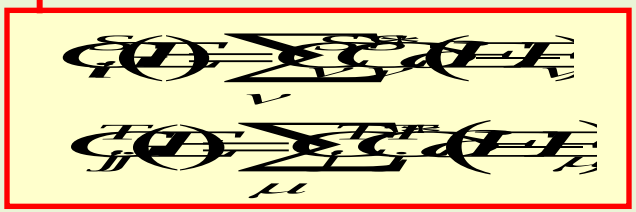
(W tip: 6s orbital)

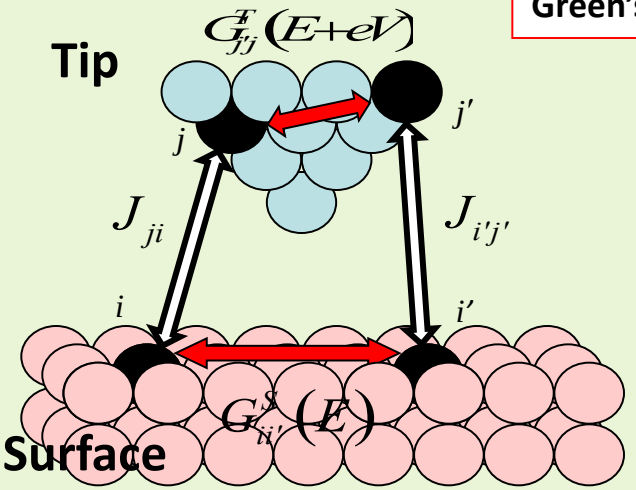
Simulation of STM image



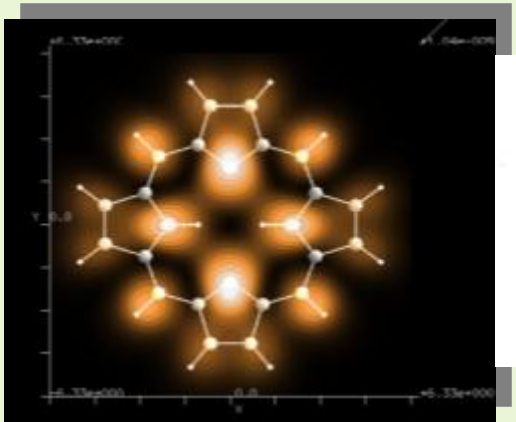
Green's function | The tunneling matrix element

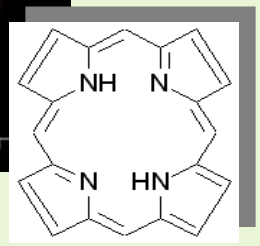
DFTB Calculation



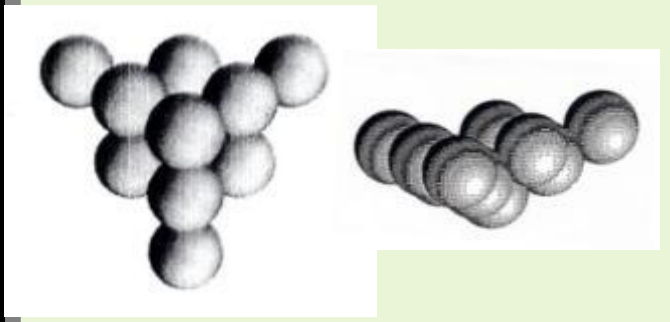


LDOS





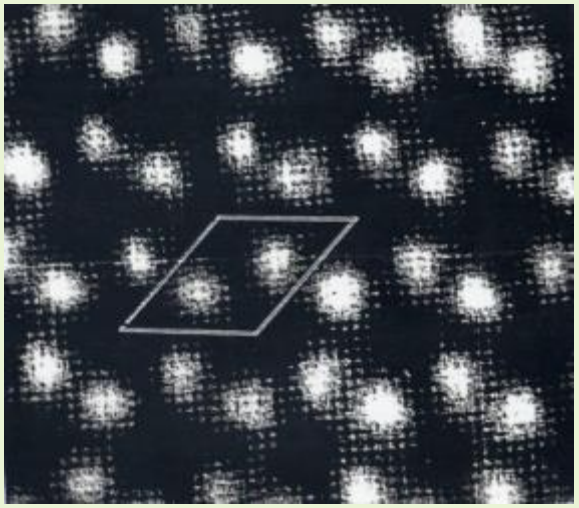
W_{10}[111] tip model



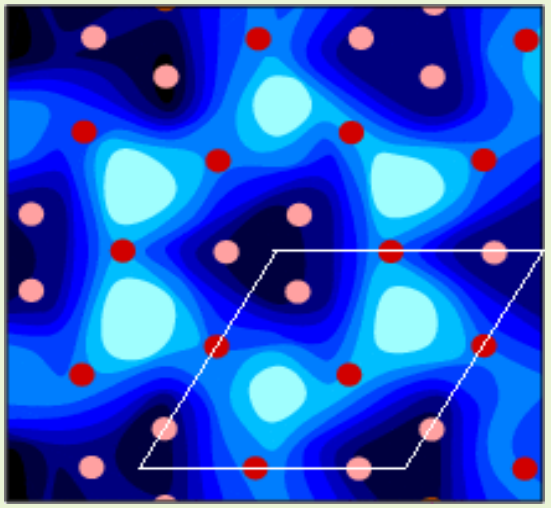
What does SPM see and how does SPM see.

In the case of the surface of Si $\sqrt{3} \times \sqrt{3}$-Ag

STM experiment



STM theory



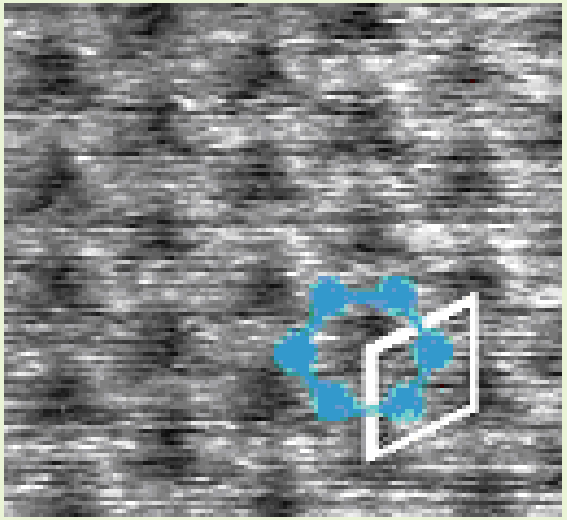
S. Watanabe, M. Aono and M. Tsukada,

Phys. Rev. B. 44, 8330 (1991)

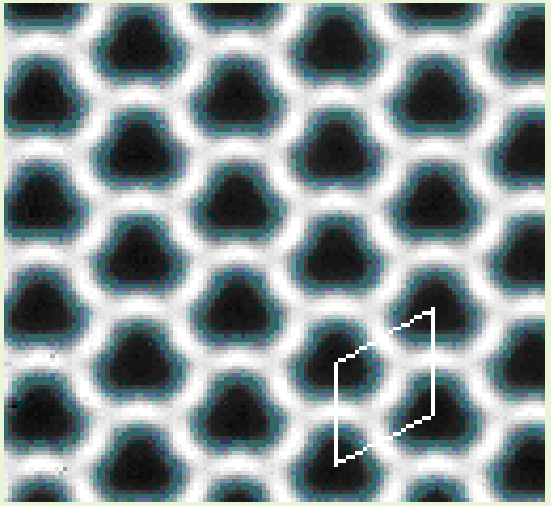
STM image and AFM image are obtained from same surface, but these are quite different.

STM image is composed of the amplitude of the unoccupied wave function.

ncAFM experiment



ncAFM theory



N. Sasaki, S. Watanabe, M. Tsukada,

Phys. Rev. Lett. 88, 046106 (2002).

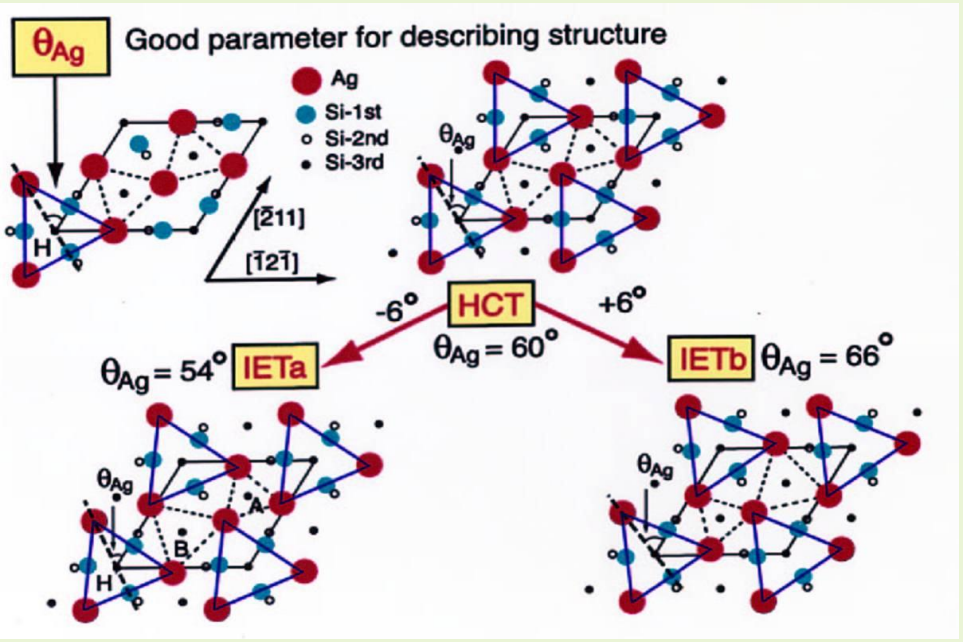
Reproduction of the AFM image is reproduced by theoretical calculation.

But...

The temperature dependability of ncAFM image of surface of Si(111)$\sqrt{3}\times\sqrt{3}$

N. Sasaki, S. Watanabe, M. Tsukada,

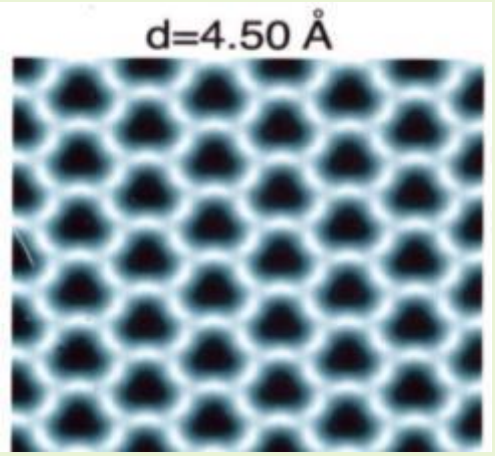
Phys. Rev. Lett. 88, 046106 (2002).



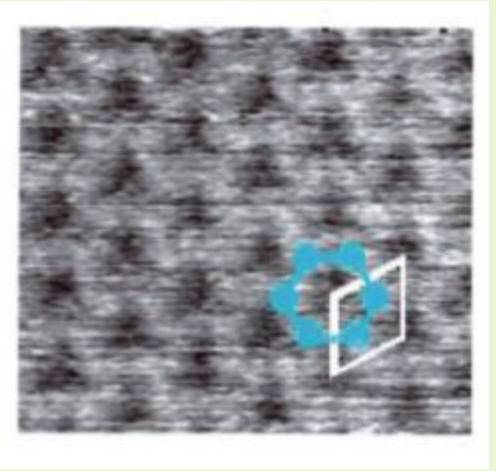
The temperature dependability can be explained by the structural fluctuation of the silver atoms in the outermost layer.

⇒ **Good agreement between the experiment and the theory**

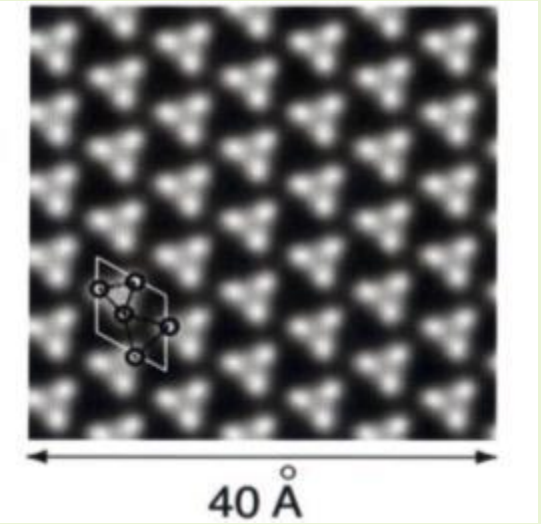
Theory



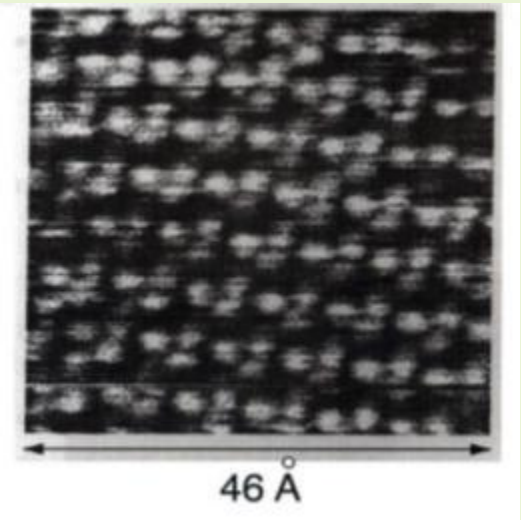
Experiment
By Prof. Morita ***T=300K***



Theory

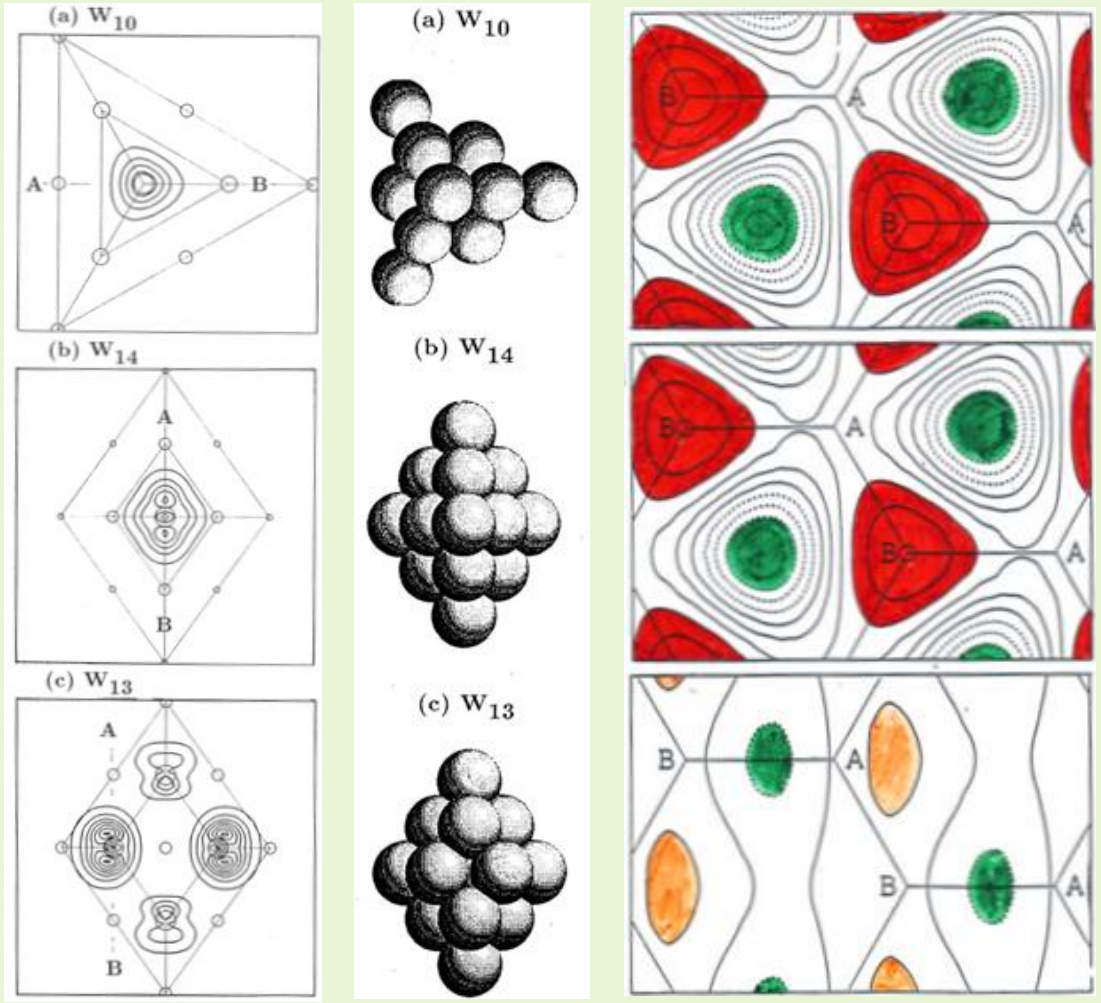


Experiment
By Prof. Morita ***T=6.2K***

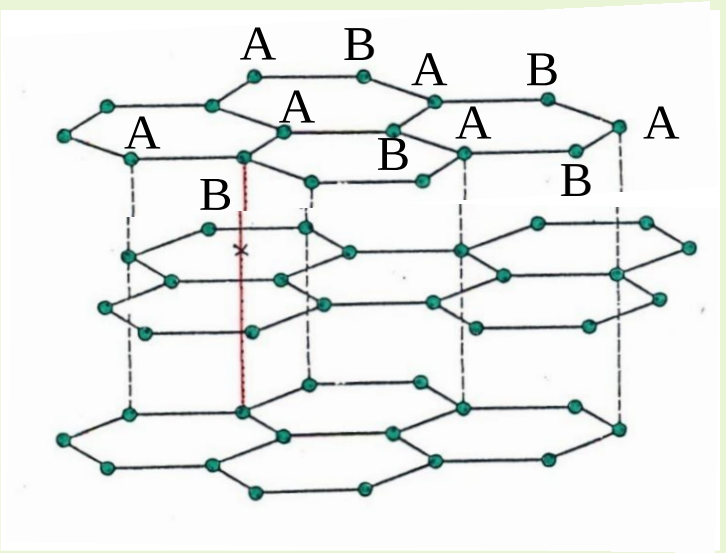


The tip-shape influence

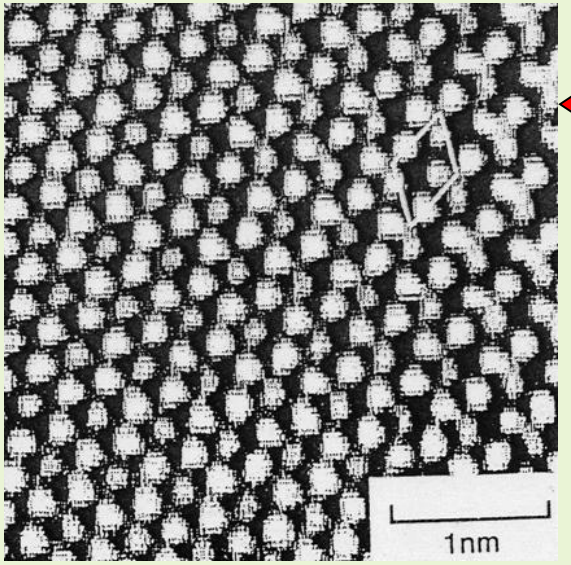
In the case of STM image of graphite



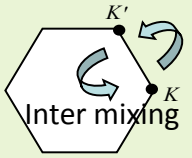
N. Isshiki, K. Kobayashi, M. Tsukada,
J. Vac. Sci. Technol. B 9(2), 475 (1991).



Nakagawa et al., Proc. Ann. Meeting of
The Phys. Soc. Jpn, (1989) 374



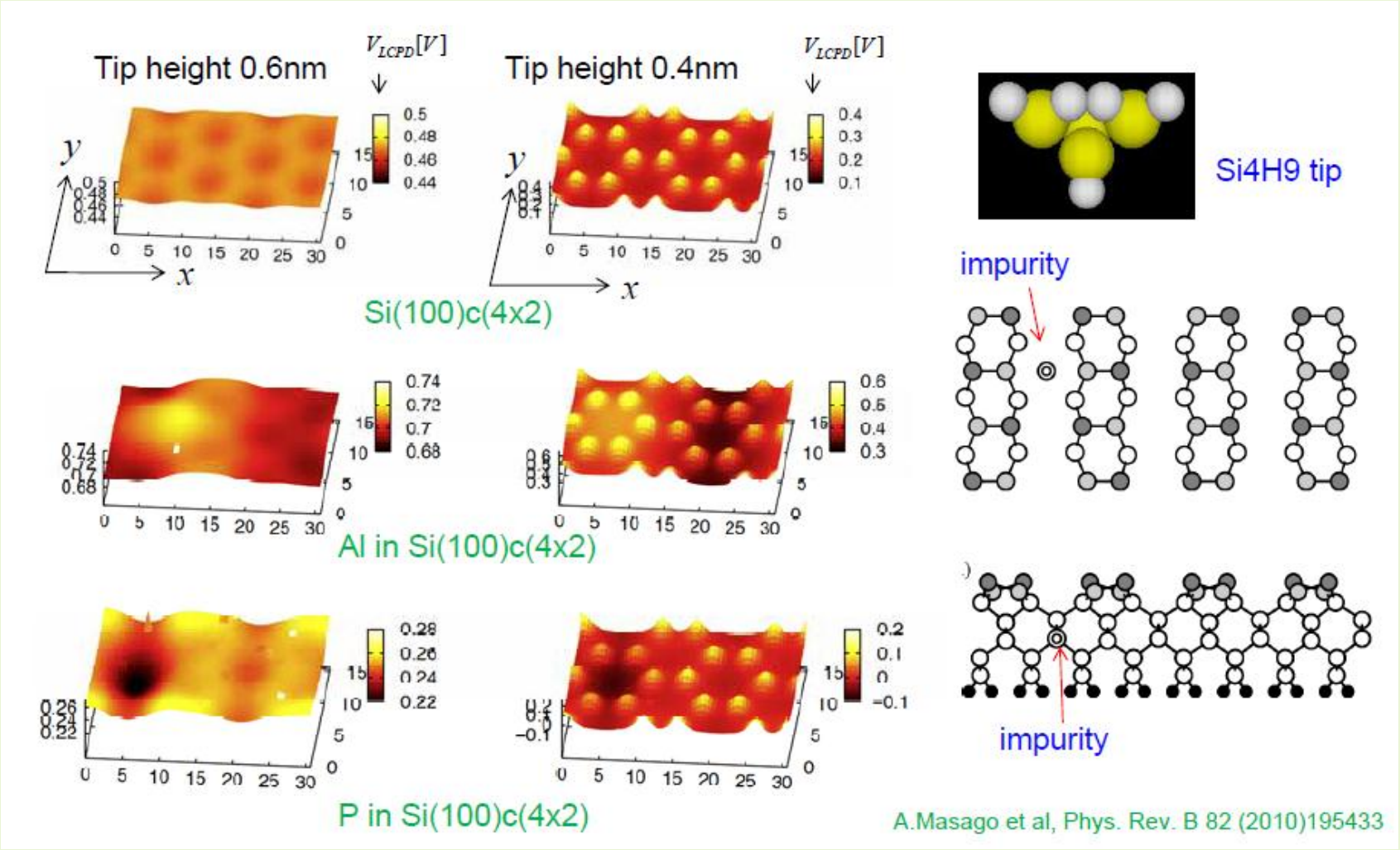
Super structure



Brilliouin Zone

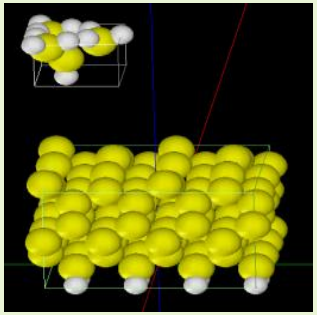
KPFM image of impurity embedded Si(001)-c(4x2) surface

DFTB -Image of distribution of local contact potential difference-



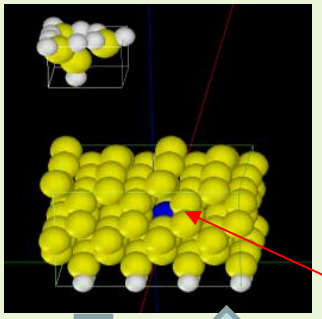
This is a result of simulation that KPFM scans the Si sample surface with an impurity. Slightly larger bright spot than the atomic scale is appeared on the surface position of the impurity, and also it can be confirmed the spot which was caused by an atom on the sample surface.

KPFM image of impurity(nitrogen atom) embedded Si(001)-c(4x2) surface



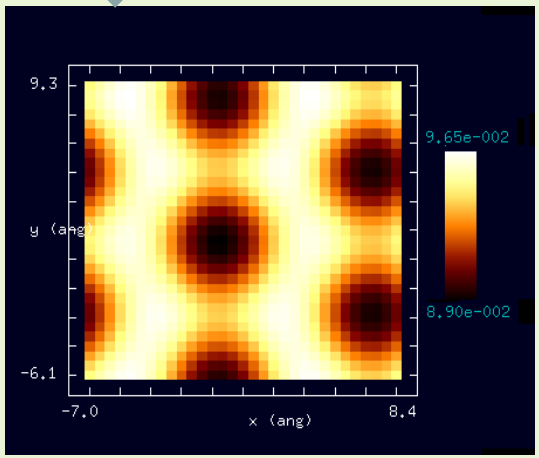
The tip: H-Si_4H_{10}
The sample surface: Si(001)-c(4x2)

Tip-surface distance: 6 Å

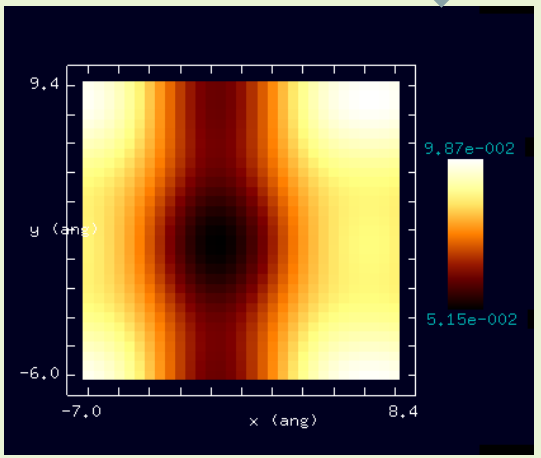


The tip: H-Si_4H_{10}
The sample surface:
Nitrogen atom is doped
Si(001)-c(4x2)

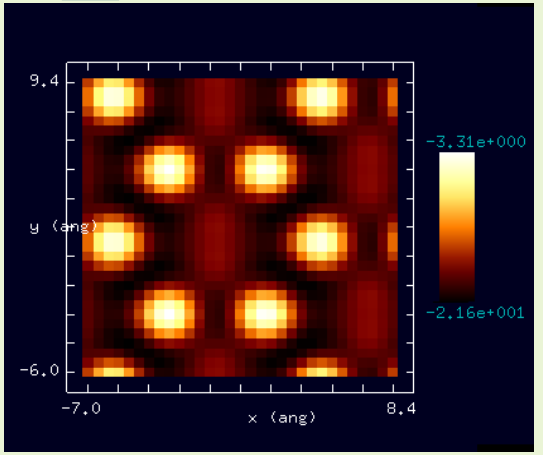
Nitrogen atom



KPFM image of a local contact potential difference
Nitrogen atom is not doped.



KPFM image of a local contact potential difference
Nitrogen atom is doped.
Nitrogen by doping,local contact potential is shifted negative.

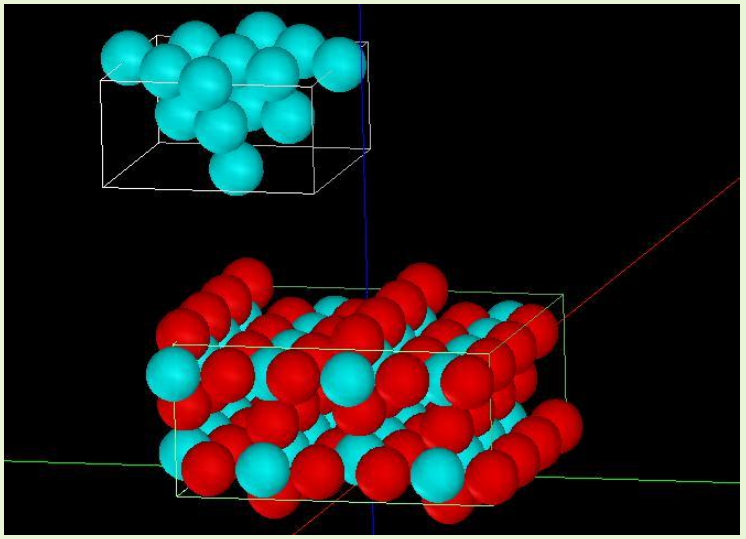


AFM frequency shift image
Nitrogen atom is doped.
Frequency shift image reflects the height of atoms.

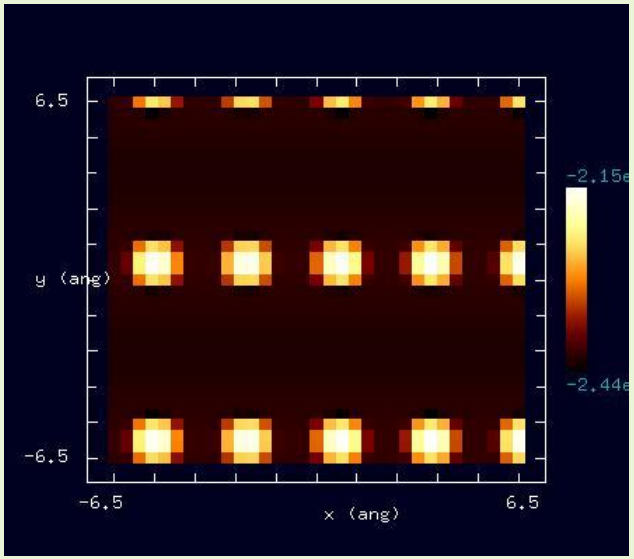
The LCPD image of a TiO_2(110) surface

DFTB The simulation of the LCPD image of a TiO2(110) surface by the KPFM.

The tip:	Pt_{14}
The sample surface:	TiO_2(110)



The tip model and the sample model

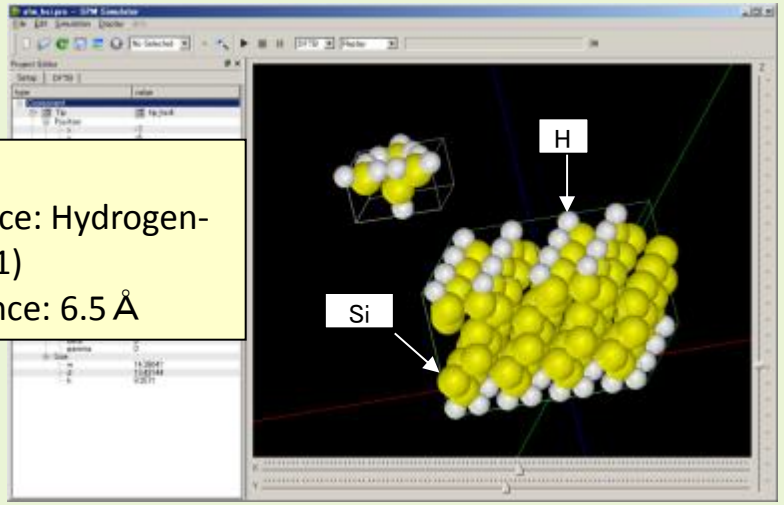


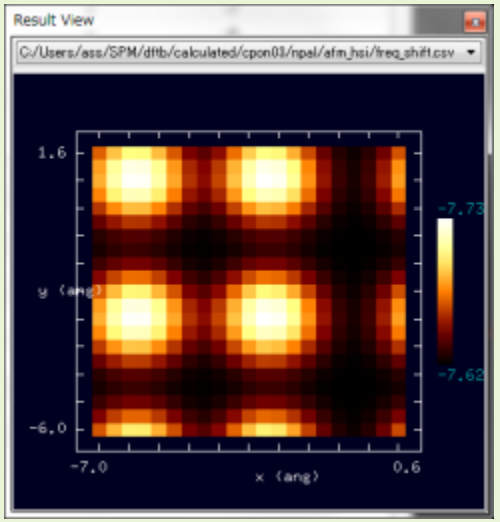
Result of the simulation of the LCPD image

The case examples of frequency shift AFM image and KPFM image

DFTB Simulation of frequency shift image

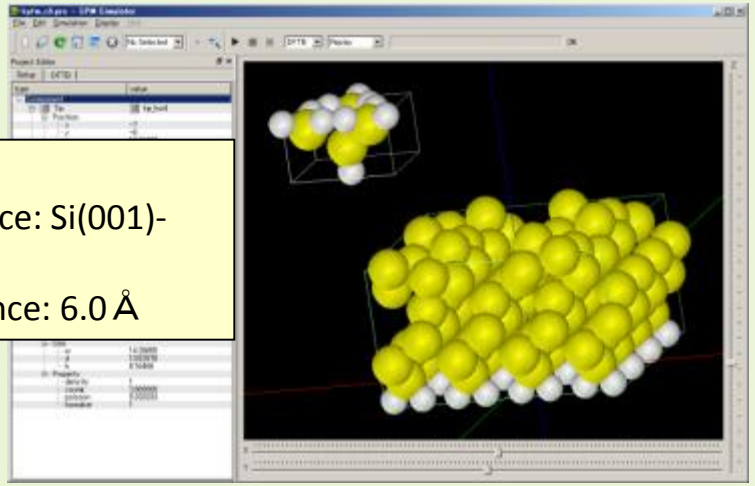
The tip: Si_4H_{10}
The sample surface: Hydrogen-terminated Si(001)
Tip-sample distance: 6.5 Å

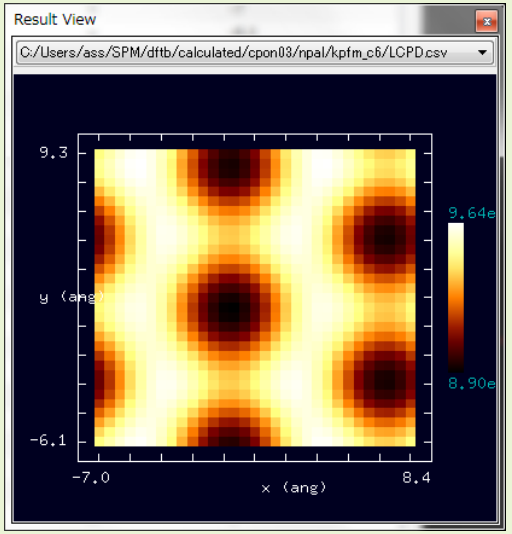




DFTB Simulation of contact potential difference image

The tip: Si_4H_{10}
The sample surface: Si(001)-c(4x2)
Tip-sample distance: 6.0 Å





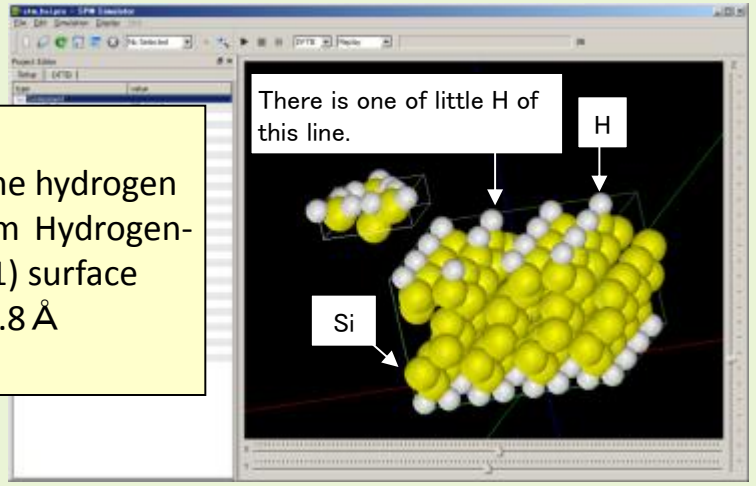
We can see the region with the large potential difference. This region coincides with the lines connecting the up dimer Si atoms.

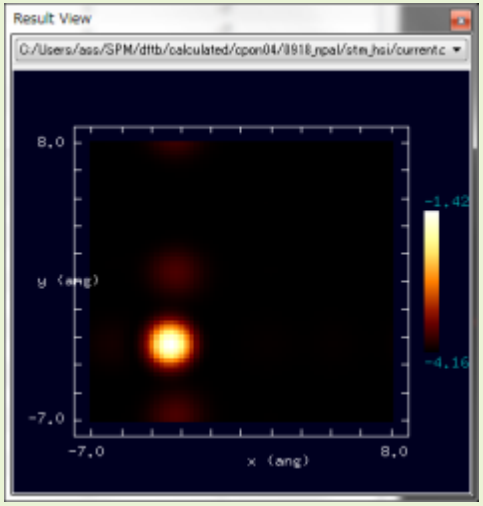
The case examples of the Scanning Tunneling Microscope and the Scanning Tunneling Spectroscopy

DFTB

Simulation of Scanning Tunneling Microscope (STM)

The tip: Si_4H_9
The sample surface: one hydrogen eliminated surface from Hydrogen-terminated Si (001) surface
Tip-surface distance: 3.8 Å



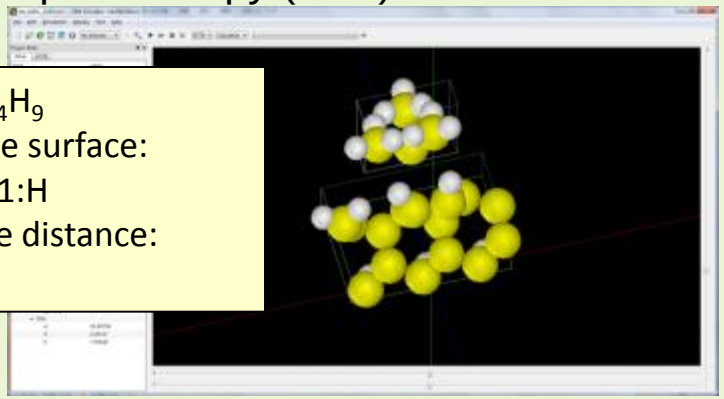


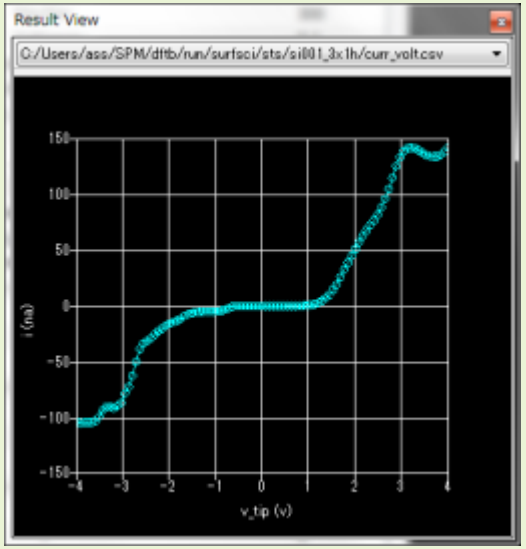
There is a dangling bond at the hydrogen- eliminated position, then this is read that a large current flows.

DFTB

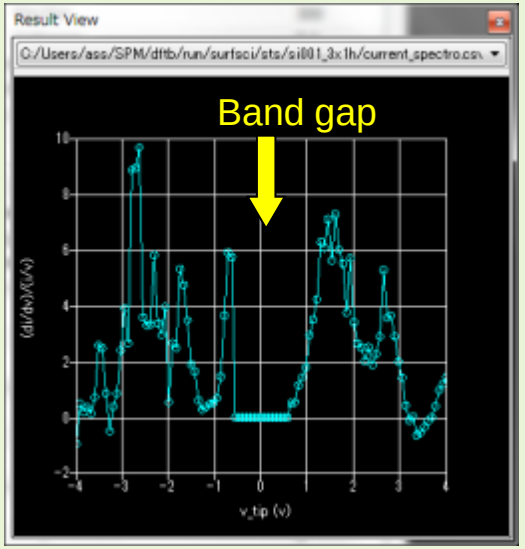
Simulation of Scanning Tunneling Spectroscopy (STS)

The tip: Si_4H_9
The sample surface: Si(001)-3x1:H
Tip-surface distance: 3.4 Å





I-V characteristic curve



(dI/dV)/(I/V) vs. V

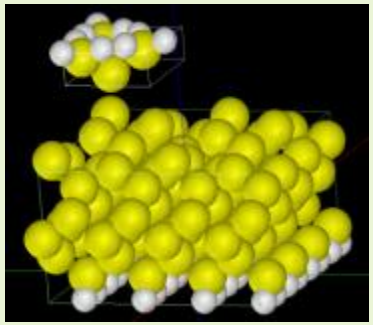
The voltage V of the horizontal axis is the tip bias compared to the sample one.

The observation and the simulation of Si(001)-c(4x2) surface by STM

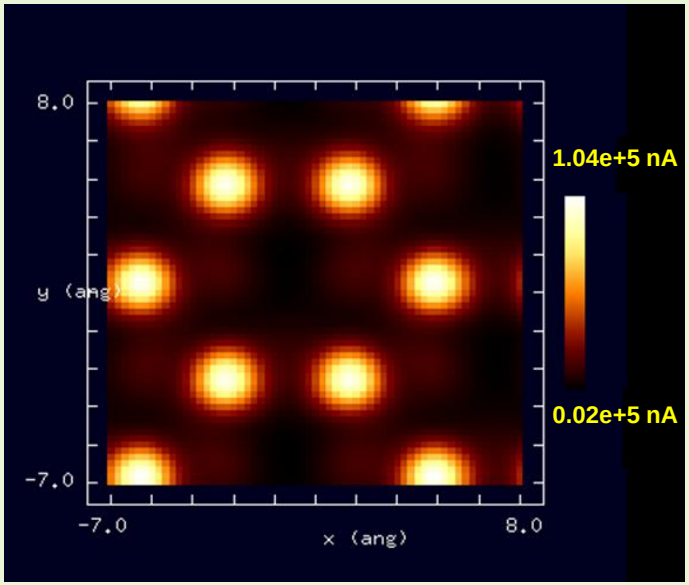
DFTB

The tip/sample model

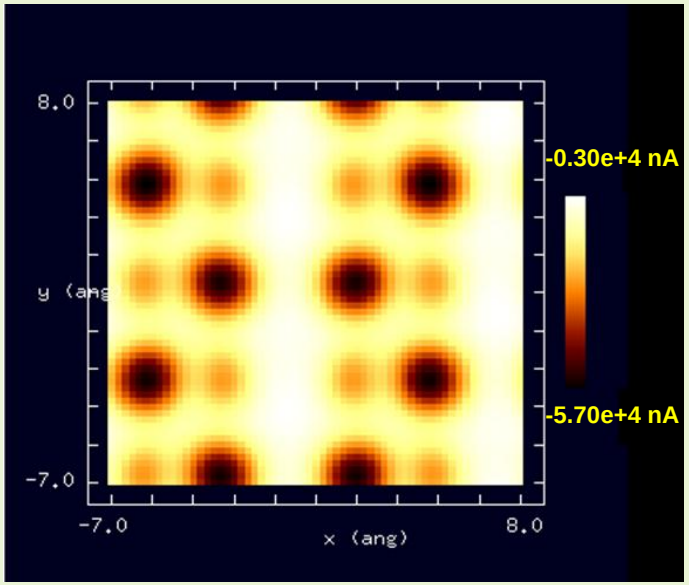
Tip: Si_4H_9
The sample surface:
Si(001)-c(4x2)
Tip-sample distance: 2.32 Å



Computed result of STM image



Bias voltage +1.0V



Bias voltage -1.0V

Honeycomb structure is inverted by the bias.

experiment

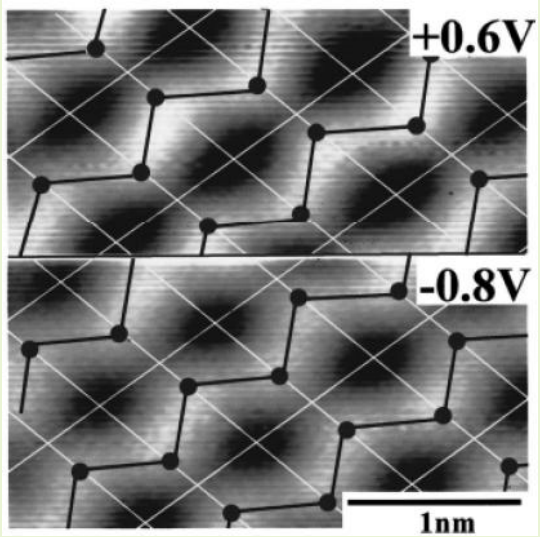


Image of tunneling current of Si(001) surface

It is known that the honeycomb structure is inverted by the sign of the bias.

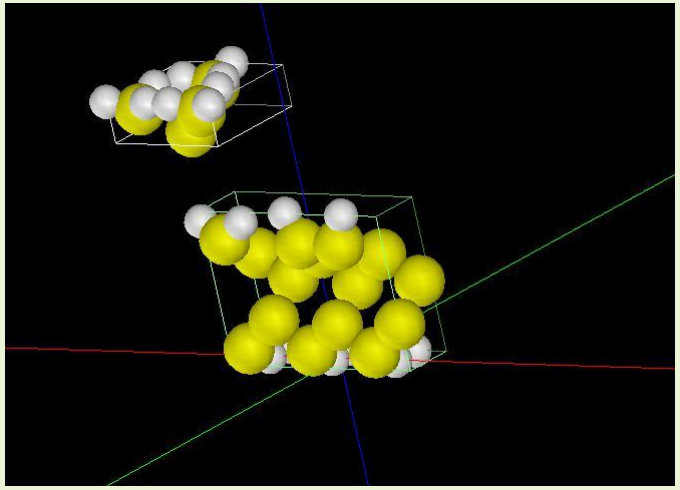
K. Hata, S. Yasuda, and H. Shigekawa, Phys. Rev. B **60**, 8164 (1999).

similarity

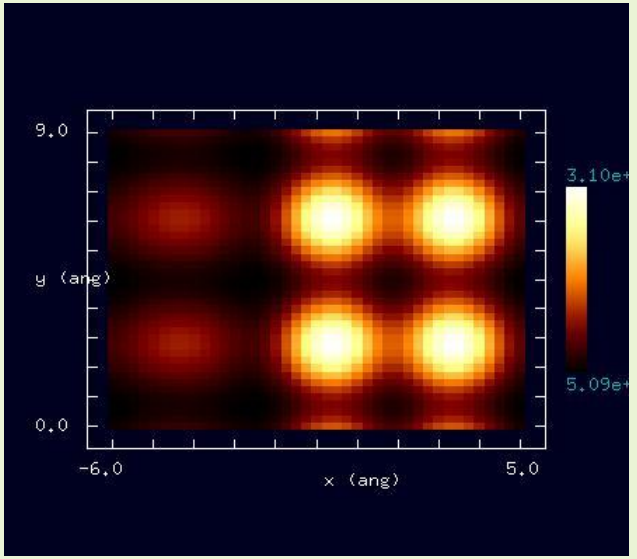
The tunneling current image of a Si(001)-3x1:H surface

DFTB The simulation of the tunneling current image of a Si(001)-3x1:H surface by the STM mode.

The tip:	Si_4H_9
The sample surface:	Si(001)-3x1:H
Tip-surface distance:	3.4 Å



The tip model and the sample model



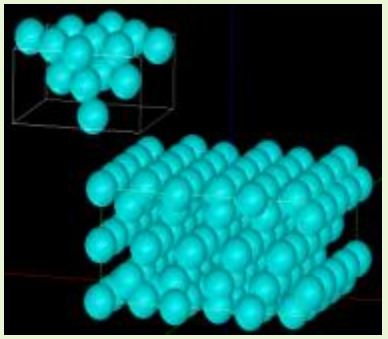
Result of the simulation of the tunneling current image

The observation and simulation of Au(001) reconstructed surface by STM

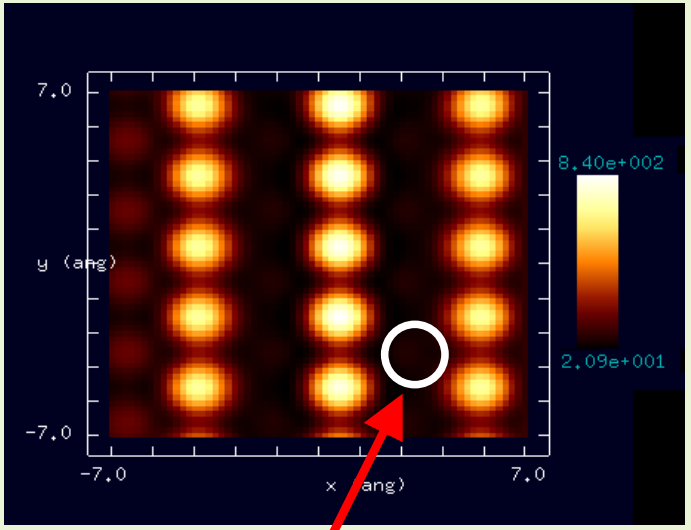
DFTB

The tip/sample model

The tip: Au_{14}
The sample surface: Au(001)-5x1 reconstructed
Tip-surface distance: 4 Å
Bias voltage (tip voltage): +0.7 V



Computed result of STM image

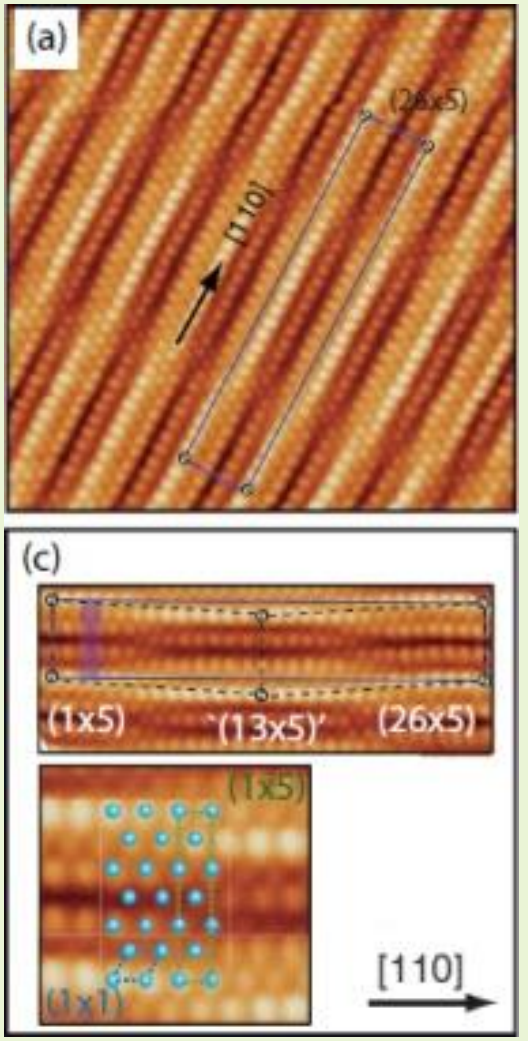


In spite of the existence of an atom, current does not flow so much.

Charge transfer occurs.

similarity

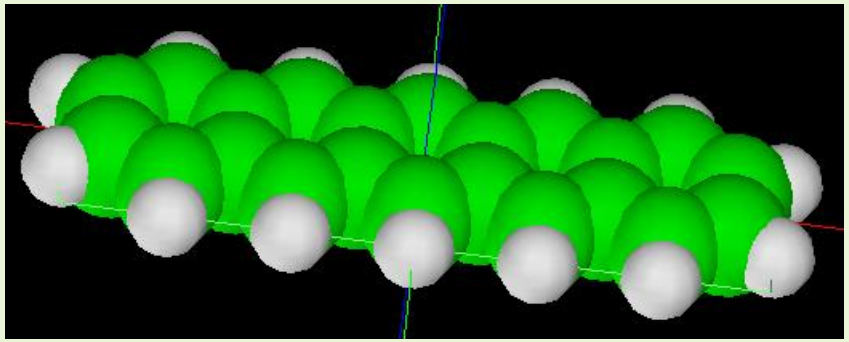
Experiment



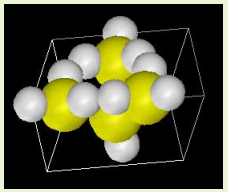
S. Bengió *et al.*, Phys. Rev. B **86**, 045426 (2012).
Au(100)-26x5 reconstructed

The observation and the simulation of pentacene molecules by AFM and STM

The tip:
Si_4H_{10} (for AFM, KPFM)
or Si_4H_9 (for STM)
The sample:
Pentacene molecule

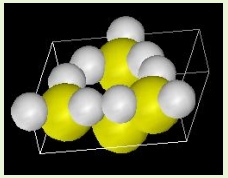


Pentacene



Si_4H_{10}

The tip for AFM, KPFM



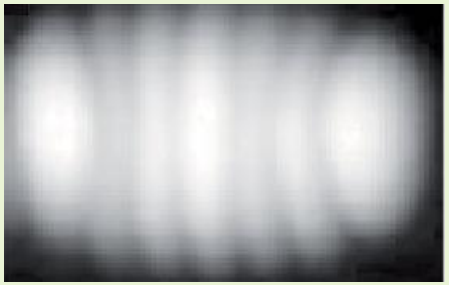
Si_4H_9

The tip for STM

Measured images

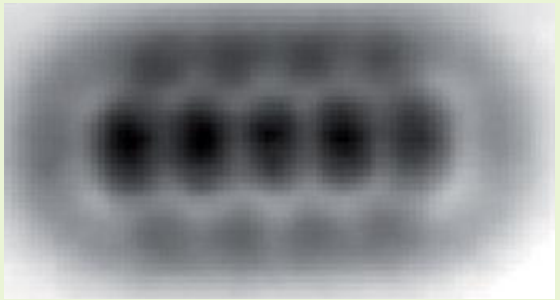
STM HOMO

Phys. Rev. Lett. 94, 026803 (2005)



STM LUMO

Same as on the left

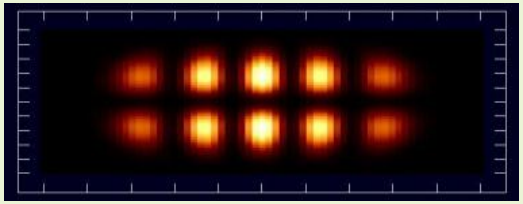


NC-AFM

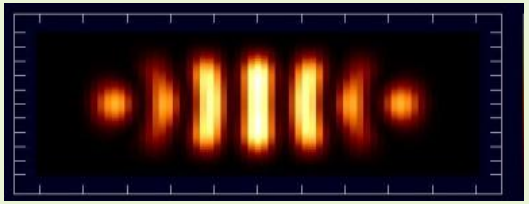
Science 325, 1110–1114 (2009)

DFTB

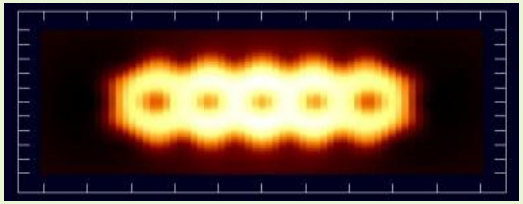
Simulated images



STM tip-sample distance: 4.0 Å
The tip bias voltage: +1.0V



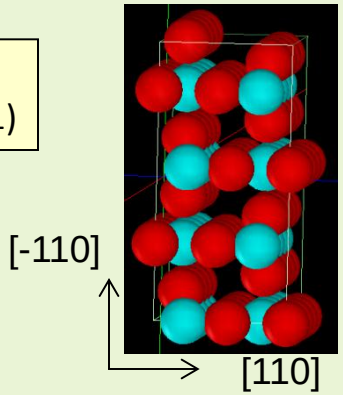
STM tip-sample distance: 4.0 Å
The tip bias voltage: -1.0V



AFM tip-sample distance: 4.0 Å

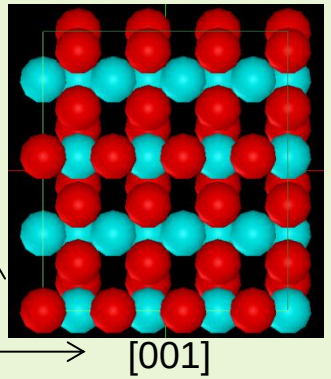
The observation and the simulation of TiO_2(110) surface by AFM and KPFM

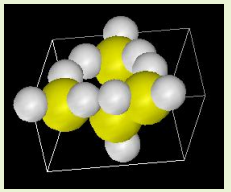
The tip: Si_4H_{10}
The sample: TiO_2(110)-(1x1)



$Ti_2O_2(OH)_2$

Oxygen of the highest position

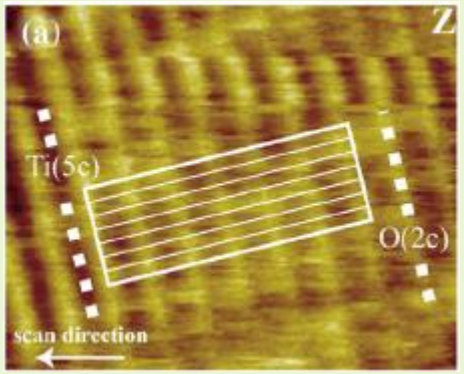




Si_4H_{10}

The tip

Measured images



AFM

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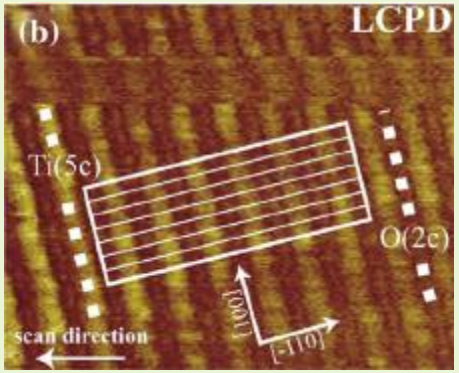
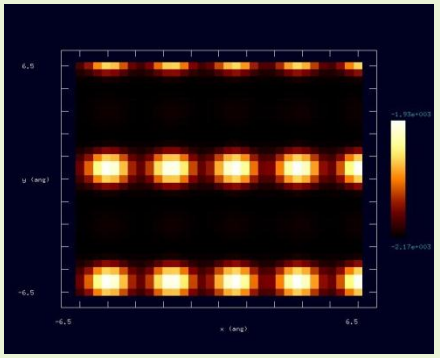
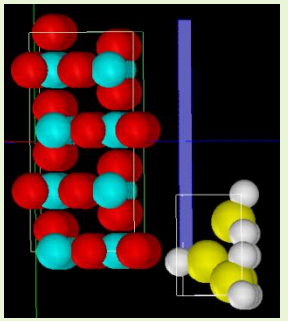
KPFM

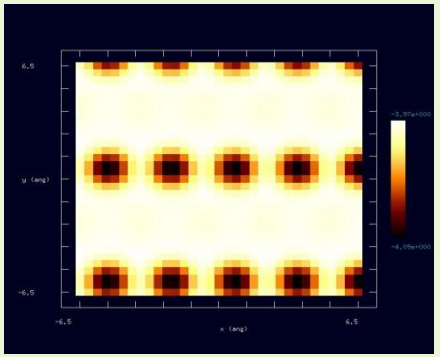


DFTB

Simulated images



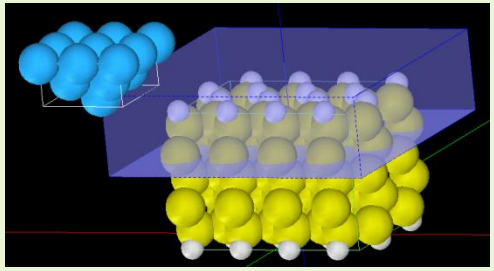




AFM Tip-sample distance: 3.5 Å

KPFM Tip-sample distance: 2.5 Å

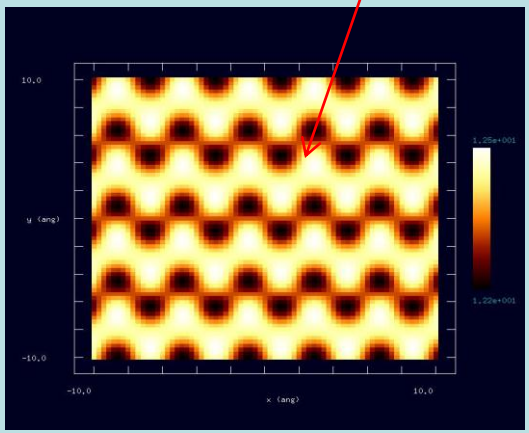
【DFTB】Constant current STM image of Si(110):H



Tip: W_{14}
Sample surface: hydrogen terminated Si(110) surface
Calculation mode: constant current STM

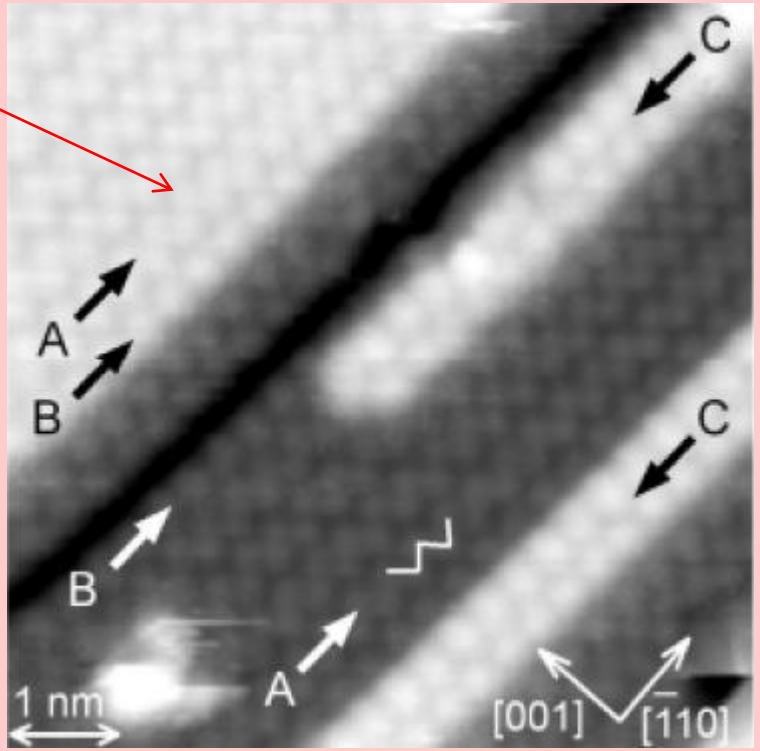
Zigzag chains in the experimental image is reproduced.

Simulated result



tip bias: +2.0V
current set point: 2000nA

cf. Experiment



Appl. Phys. Lett. 85, 6254 (2004)

sample bias: -2.0V
current set point: 0.3nA

Sample Modeling

SetModel

Inputting crystal data, create a sample model of any size

↓

Remove, copy, move an atom and change the element.

↓

Hydrogenate, generate of MM3 force field parameters.

↓

Save as the suitable format for each solvers.

How to make a graphite thin film with a defect.

Crystal data

The space group number:194

The lattice constants:

a = 2.464 Å

b = 6.711 Å

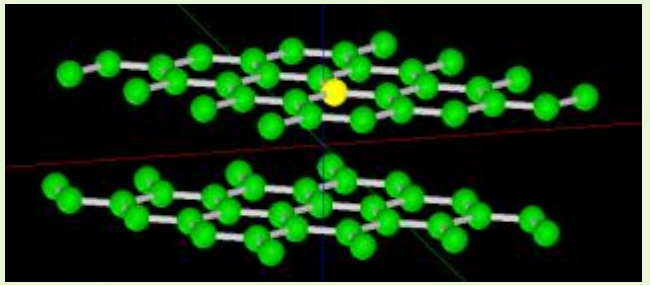
Fractional coordinate: C (0, 0, 1/4)

C (1/3, 2/3, 1/4)

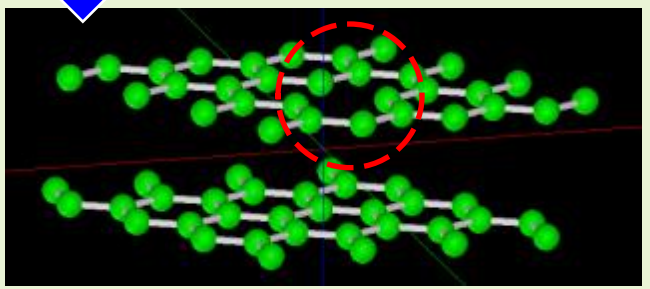
Direction and size

Miller index: (0 0 1)

Size of lattice: (4, 4, 1)



Select an atom and remove it.



Create MM3 force field parameters

Save as txyz format

Save as xyz format

CG MD GeoAFM FemAFM DFTB

Sample Modeling

SetModel

Inputting crystal data, create a sample model of any size

Remove, copy, move an atom and change an element.

Hydrogenate, generate of MM3 force field parameters.

Save as the suitable format for each solvers.

How to make a tip model of a silicon cluster.

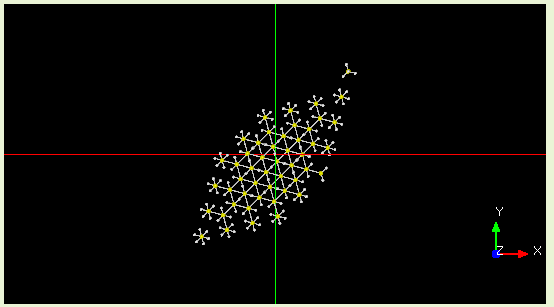
Crystal data

The space group number: 227
The lattice constants:
a = 5.4 Å
Fractional coordinate:
Si (0, 0, 0)

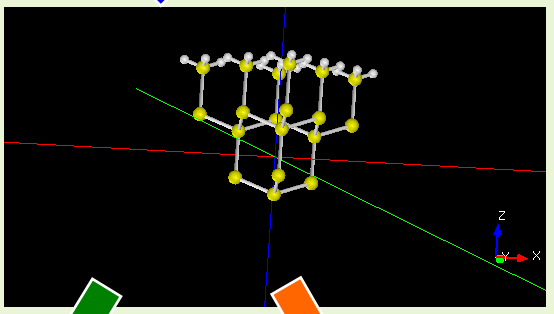
Direction and size

Miller index: (1 1 1)
Size of lattice:(2, 2, 3)

Hydrogenate the dangling bounds



Cut off the useless parts to make an apex structure with a sharp top.



Create MM3 force field parameters

Save as txyz format

Save as xyz format

CG MD

GeoAFM FemAFM

DFTB

Sample Modeling

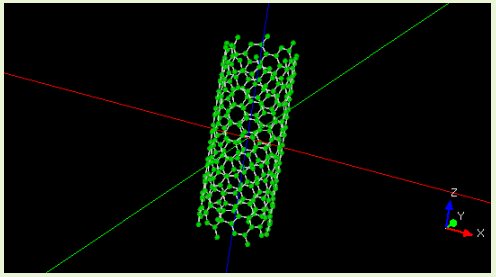
SetModel

How to make a carbon nanotube or its derivatives.

Single-wall nanotube

Input data

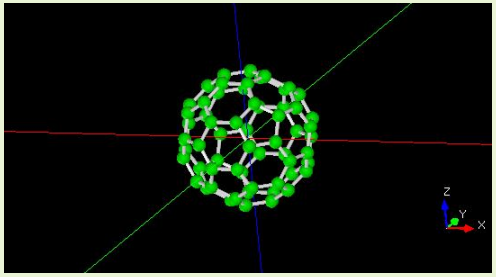
mode: swcnt
Chiral index: (8, 6)
Number of unit cell: 1



Fullerene

Input data

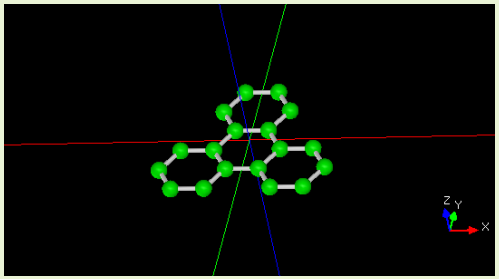
mode: fuller
Chiral index: (5, 5)
Number of unit cell: 1



Graphene sheet

Input data

mode: sheet
Chiral index: (20, -10)
Number of unit cell : 1



Capped carbon nanotube

Input data

mode: capped
Chiral index: (10, -5)
Number of unit cell: 8