To researchers of the SPM in university, public institutes, and private companies

We prepare typical examples of simulations for your research fields as follows:
The fields of inorganic compounds and metals:
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Inorganic_Organic_Bio.htm
The fields of organic compounds and bio-related materials:
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Organic_Bio.htm

Please tell us which solver you want to use. Please tell us which type you need, the standard type or the professional type.
(1) You can enjoy free trail use of solvers for three months.
(2) You can consult us about a method for purchase and other questions in the following web sites:
▪ **https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_purchase_process_ver2.pdf**
▪ **https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_User_Support_Manual_v03s_171029.pdf**
Please feel free to contact us: spm-simulator-howto@aas-ri.co.jp

The SPM simulator
The web seminar

We prepare around 600 case examples of simulations for your convenience.
https://www.aasri.jp/pub/spm/pdf/catalog/CaseExamplesofCalculation_eng.pdf

Advanced Algorithm & Systems Co., Ltd.and our partner companies

The SPM simulator enables you to compare experimental results and numerical simulations. It is based on the tight-binding density functional theory. We provide opportunities to learn how to use the SPM simulator for you.
We welcome researchers in the following fields:

a. People who want to enjoy free trial use and learn how to use the simulator
b. Researchers who use the simulator from 2011 and want to update it
c. Researchers in the field of bio-related materials, polymers, organic semiconductors, organic and inorganic materials, semiconductors, and surface science
d. People who are interested in contact problems for viscoelastic bodies, soft matters, viscoelastic systems, surface water, SPM experiments in the liquid environment, and the tapping mode of AFM
e. Using 69 atoms for the DFTB solver, you can simulate experiments of STM, STS, AFM, and KPFM with various organic and inorganic compounds, semiconductors, and metals in a very short time. If you have an old version of the SPM simulator, we give you a new one for the first year. You only have to pay the charge from the second year.
f. Researchers who can give numerical data obtained by using the SPM simulator to us. If you allow us to disclose your numerical results on our home page, we offer free trail use of the SPM simulator for one year to you.

You can select one of the following three methods for purchasing the SPM simulator.

(1) Experienced researchers of the SPM
After reading the Web seminar and the guidebook for the SPM simulator, you can enjoy free trial use of the SPM simulator for three months. Please let us know your own problems that you want to simulate. You and we can share advanced knowledge about the SPM. After you evaluate our simulator, you enter into a contract of purchase of the SPM simulator with us. If you have a question, please make a contact with us by e-mail. (spm-simulator-howto@aas-ri.co.jp)
https://www.aasri.jp/pub/spm/pdf/SPM_exploit_future.pdf
https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_purchase_process_ver2.pdf
https://www.aasri.jp/pub/spm/about_spm.html
https://www.aasri.jp/pub/spm/pdf/spm_howtouse.pdf
https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_User_Support_Manual_v03s_171029.pdf

(2) Beginners of the SPM
You can learn how to use the SPM simulator by reading the Web seminar and the guidebook of the SPM simulator. You can refer to case examples that we prepare. Consulting our engineers about technical problems, you will obtain practical skills for simulation. After these processes, you enter into a contract of purchase of the SPM simulator with us. If you have a question, please make a contact with us by e-mail. (spm-simulator-howto@aas-ri.co.jp)
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Organic_Bio.htm
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Inorganic_Organic_Bio.htm
Please pay attention to the following facts:
While you are learning how to use the SPM simulator, you can enjoy the free trial use of the simulator.
Moreover, we can offer technical supports to you with charging a fee.

(3) The other researchers who are not included in the above cases
We prepare various options for contracts of purchase of the SPM simulator. If you purchase or lease the SPM simulator, we can apply rules flexibly according to your requests.
If you have a question, please make a contact with us by e-mail. (spm-simulator-howto@aas-ri.co.jp)

A program of the web seminar

Under the instruction of Professor Masaru Tsukada in Tohoku University Advanced Institute for Materials Research (AIMR), we have developed the following software:
https://www.aasri.jp/pub/demo/application/SPM_PressRelease.pdf

The theoretical background of the SPM simulator and its multi-purpose simulations
https://www.aasri.jp/pub/spm/pdf/spm16720101125.pdf
Theoretical simulations of AFM in the liquid environment and contact problems for viscoelastic bodies
https://www.aasri.jp/pub/spm/pdf/AFM_theory_eng.pdf
The present state and future problems of the SPM simulator
https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_Simple_Introduction_2017Dec_V6.pdf
Simulations of AFM in the liquid environment using the DLVO theory
https://www.aasri.jp/pub/spm/pdf/DLVO_national_project_20171122a.pdf
https://www.aasri.jp/pub/spm/pdf/SPM_progress_report_meeting20180224_document.pdf

A program of the web seminar

The SPM simulator: the software for comparing experimental results and numerical simulations The SPM simulator is developed in Japan for worldwide use.

Using the SPM simulator, we can share common interests and knowledge in research activities.
Whether you are skillful users or beginners of the SPM simulator, we, namely Advanced Algorithm and Systems, hope to collaborate with you.
https://www.aasri.jp/pub/spm/pdf/catalog/imagepamphlet/SPM_ApplicationField.pdf

You can find important information for performing simulations with the SPM simulator on our web sites according to your research field.

We, namely Advanced Algorithm and Systems, hope to collaborate with you.
You and we share results of simulations, and we want to disclose the knowledge obtained through the collaboration to the world.

We want to establish a knowledge-based infrastructure of the SPM simulator with you.

We show typical applications of the SPM simulator for various fields in the following web page. Please click an item where your research topic is includes.
https://www.aasri.jp/pub/spm/SPM_simulator_application_examples.html
In this web page, we make up the list that has eight research fields.
You can find your research area in this list.
Clicking the item, you can learn how to make use of the SPM simulator for your own research activities.

A program of the web seminar

As shown in the previous page, we present eight research fields to you.
Particularly, we pay attention to the fields of Inorganic_Organic_Bio and Organic_Bio.

Please tell us your research fields and research topics that you are interested in.
We provide you with the SPM simulator.
Using this simulator, you can compare your own experimental results and numerical data obtained by the simulation.
Thus, you can derive new knowledge about experiments of the SPM.
We want to collaborate with you on various research topics and share experimental data with you, because we hope to disclose experimental data for promoting our software as a convenient tool for researchers in the field of the SPM.

We divide research fields of the SPM into two areas.
The first one is Inorganic_Organic_Bio.
The second one is Organic_Bio.

According to the above classification, we show you typical examples of the numerical simulations.
Typical examples of the SPM simulator in the field of Inorganic_Organic_Bio:
https://www.aasri.jp/pub/spm/WebSeminar/SPM_Simulator_Seminar_sample_Inorganic_Organic_Bio.htm
Typical examples of the SPM simulator in the field of Inorganic_Organic_Bio:
https://www.aasri.jp/pub/spm/WebSeminar/SPM_Simulator_Seminar_sample_Organic_Bio.htm

A program of the web seminar

For experts of the SPM simulator:
https://www.aasri.jp/pub/spm/pdf/catalog/imagepamphlet/SPM_ApplicationField.pdf
Typical examples of the SPM simulation classified according to fields of application
https://www.aasri.jp/pub/spm/SPM_simulator_application_examples.html
For beginners:
https://www.aasri.jp/pub/spm/pdf/SPM_ApplicationField_for_beginners.pdf

We present two databases to you.
The first one is a database for case studies of simulations classified according to the fields of application.
The second one is a database for case studies of simulations for each solver.
https://www.aasri.jp/pub/spm/pdf/catalog/imagepamphlet/SPM_ApplicationField.pdf
https://www.aasri.jp/pub/spm/SPM_simulator_application_examples.html
https://www.aasri.jp/pub/spm/pdf/SPM_ApplicationField_for_beginners.pdf
https://www.aasri.jp/pub/spm/pdf/case_examples_20170223/spm_case_examples.pdf
We prepare manuals of the SPM simulator in the following web page:
https://www.aasri.jp/pub/spm/SPM_movie.html

A program of the web seminar

Now, we are improving the SPM simulator, so that experimental researchers of the SPM can utilize the simulator effectively.

So far, the SPM simulator calculates the SPM images from the structural data of the sample and the tip and the physical parameters given as input data.
However, according to this method, the experimental user cannot make use of their experimental data as input of the SPM simulator.
Although the user have their own image data of the SPM, they cannot process their own experimental results using the simulator.

We are developing the new solver, which extracts the physical quantities from experimental results.
In other words, we are intend to accomplish the solver that treats the inverse problems.
Using this solver, the user can obtain Young's modulus and surface tension of the sample from experimental results of the frequency shift and the phase shift, for example.

So far, we have been only paying attention to the direct problems, that is to say, the solver have obtained SPM image from structural data of the tip and the sample and the physical parameters given as input data.
However, from now on, we change the concept of the solvers and we develop a new solver for treating the inverse problem.

Please consider introducing our new solver that examine the inverse problems.

A program of the web seminar

Examples of simulations with the SPM simulator
http://www.aasri.jp/pub/spm/pdf/case_examples_20170223/spm_case_examples.pdf

You can find an example of a simulation that resembles yoiur own problem in the following two databases.
The first one is a database for case studies of simulations classified according to the fields of application.
The second one is a database for case studies of simulations for each solver.
https://www.aasri.jp/pub/spm/pdf/catalog/imagepamphlet/SPM_ApplicationField.pdf
https://www.aasri.jp/pub/spm/SPM_simulator_application_examples.html
https://www.aasri.jp/pub/spm/pdf/SPM_ApplicationField_for_beginners.pdf
https://www.aasri.jp/pub/spm/pdf/case_examples_20170223/spm_case_examples.pdf

We prepare manuals of the SPM simulator in the following web page.
You can find a case study which gives you suggestions about how to use the SPM simulator to your own problem.
https://www.aasri.jp/pub/spm/SPM_movie.html

A program of the web seminar

The help menus for beginners of the SPM simulator are given by the following web pages.
Perspective views of the operational navigation system for the SPM simulator:
https://www.aasri.jp/pub/spm/pdf/spm_howtouse.pdf
https://www.aasri.jp/pub/spm/about_spm.html
The manuals of the SPM simulator for beginners:
https://www.aasri.jp/pub/spm/pdf/DFTB_BAND_PHASE0.pdf
https://www.aasri.jp/pub/spm/mail/mail20161102.html
https://www.aasri.jp/pub/spm/mail/mail20170811_2.html
https://www.aasri.jp/pub/spm/mail/mail20170228.html

We would like to tell you how to utilize the manuals of the SPM simulator.
We can provide you with services, such as supporting you for learning how to use the SPM simulator in direct.
We prepare both charged and free supports.

The SPM world

The SPM simulator is the AFM simulator for soft matters and bio-related materials.
This simulator can compare experimental images and results of calculations at the same time.
Our simulator is the world's first one and made in Japan.

The SPM simulator can analyze viscoelastic contact mechanics for soft matters and bio-related materials.
The DFTB solver can simulate 69 kinds of elements and examine organic compounds, organic semiconductors, inorganic semiconductors, and metals.
You can use the SPM simulator for generating input data for the PHASE/0.

The SPM simulator can compare and investigate experimental images and results of calculations at the same time on the same platform.
The human body is made from twenty trillion cells.
The cell is constructed by molecules, whose dynamics is understood by statistical mechanics.
You can study polymers and proteins in the human body using the SPM simulator.
The SPM simulator can contribute to research activities in the medical and pharmaceutical fields.

The SPM world

The SPM simulator is world's first AFM simulator for soft matters and bio-related materials.
Our simulator can compare experimental images and results obtained by calculations.
We offer you the SPM simulator as type 1 and type 2 package.

[Package 1]
We offer you the type 1 package according to your research fields.
You can learn how to use the SPM simulator by the web seminar.
You can enjoy free trial of use of the SPM simulator for three months.
After you and we recognize your own problems for research activities and share technical knowledge, we enter into a contract for purchasing the SPM simulator.

you can consult us about technical problems before entering into a contract.
The web seminar for the SPM simulator
You can find typical examples of simulations that resemble your own problems.
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Organic_Bio.htm
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Inorganic_Organic_Bio.htm

The SPM world

We prepare a list on which research topics are arranged according to market segments. You can find which solver is suitable for your market segment from this list.

https://www.aasri.jp/pub/spm/pdf/catalog/imagepamphlet/SPM_ApplicationField.pdf

We prepare a list on which functions of the SPM simulator are arranged according to the typical examples of simulations. You can find which solver is suitable for your own problem from this list.

https://www.aasri.jp/pub/spm/SPM_simulator_application_examples.html

The SPM world

When you enter into a contract for purchasing the SPM simulator, we ask you to pay 10 percent of the total payment as the deposit.
You can enjoy free trial of use of the SPM simulator for three months.
During the free trial, you can consult us about technical problems.
If you want to update your software as the latest version, you only have to pay the difference.

We prepare web pages, on which instructive information for beginners of the SPM simulator is described.
We also prepare input data for various simulations.
You can find a typical example of the simulation that resemble your own problem.
Thus, you do not need to make input data from the beginning.
You only have to download our input data and edit it for your own purpose.
https://www.aasri.jp/pub/spm/mail/mail20170228.html
Movies for beginners:
https://www.aasri.jp/pub/spm/SPM_movie.html

The SPM world

The operational navigation system for the SPM simulator
https://www.aasri.jp/pub/spm/assistant_eng/SPM_Simulator_assistant_top.htm
https://www.aasri.jp/pub/spm/about_spm_assistant_intro.html
SPM Interactive Information Exchanging Platform
https://www.aasri.jp/pub/spm/en/about_spm_eng.html

Please look at the top page to participate the web seminar for the SPM simulator:
https://www.aasri.jp/

[Package 2]
If you want to use the SPM simulator as soon as possible, please look at the following web pages:
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Organic_Bio.htm
https://www.aasri.jp/pub/spm/SPM_Simulator_Seminar_sample_Inorganic_Organic_Bio.htm
The web seminar for the SPM simulator
Please feel free to contact us for participating the web seminar:
spm-simulator-howto@aas-ri.co.jp

The SPM world

Information for the SPM simulator:

The web seminar for the SPM simulation

https://www.aasri.jp/

SPM Interactive Information Exchanging Platform

https://www.aasri.jp/pub/spm/en/about_spm_eng.html

The process for purchasing the SPM simulator

https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_purchase_process_ver2.pdf

A program of the web seminar

You can consult the following staff about technical problems of the SPM simulator.

Dr. Tsukada Masaru (Emeritus Professor of University of Tokyo)
<tsukada@wpi-aimr.tohoku.ac.jp>
Dr. Takahisa Ohno (National Institute for Materials Science, Nano-Theory Field, Computational Nanoscience Group, International Center for Materials Nanoarchitectonics)
<OHNO.Takahisa@nims.go.jp>
Dr. Jun Nara <NARA.Jun@nims.go.jp>
Dr. Takahiro Yamasaki <YAMASAKI.Takahiro@nims.go.jp>
Dr. Kohichiro Oyama (JAXA, Japan Aerospace Exploration Agency, President of CoLtd., Asia Space Environment Research Consortium)
<koh_ichiro@yahoo.co.jp>

You can apply the purchase of the SPM simulator by sending an e-mail to us:
spm-simulator-howto@aas-ri.co.jp
Please feel free to contact us if you have any questions.

A program of the web seminar

(1) You can confirm accomplishments of our software by looking at contents of our web sites.

(2) You can purchase the SPM simulator on the installment plan.

(3) We offer free trial use of the software to researchers in universities, engineers in private companies, experts and beginners of the SPM simulator.

https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_purchase_process_ver2.pdf

https://www.aasri.jp/pub/spm/pdf/spm_howtouse.pdf

https://www.aasri.jp/pub/spm/about_spm.html

https://www.aasri.jp/pub/spm/pdf/SPM_Simulator_User_Support_Manual_v03s_171029.pdf

We disclose scientific knowledge and information about the SPM simulator in the following web pages:

https://www.aasri.jp/pub/public/AAS_knowledge_info.html

https://www.aasri.jp/pub/top_private/area.html

Scientific information about the SPM simulator

https://www.aasri.jp/

https://www.aasri.jp/pub/spm/about_spm.html

https://www.aasri.jp/pub/spm/pdf/spm_howtouse.pdf

For the participants of the web seminar of the SPM simulator

https://www.aasri.jp/pub/spm/pdf/WebSeminar_Organic_Bio.pdf

If you want to attend the web seminar, please feel free to contact us:

spm-simulator-howto@aas-ri.co.jp

The SPM simulator

The theoretical and experimental Scanning Probe Microscope simulator

Developed by the laboratory in the Japanese university, de facto standard

## What is the Scanning Probe Microscope simulator?

- It simulates various experiments of the Scanning Probe Microscope numerically.
- It uses techniques of the continuum mechanics, the fluid dynamics, the molecular dynamics, and the density functional method.
- It can perform digital image processing on experimental data of the SPM.
- It can extract novel knowledge by comparing both simulation results and experimental results.

Differences between the SPM simulator and conventional technologies

- Only the SPM simulator can process both experimental data of the SPM and simulation data on the same platform.
- It offers continuum mechanical simulations and the AFM simulations in the liquid environment for researchers in the field of polymers and bio-related materials.
- It enables experimental researchers to perform numerical simulations with ease.
- It has a simple and excellent graphical user interface which gives you high productivity.

The world of the SPM simulator

- Target audiences of our simulator are researchers in the field of the surface science.→Please look at the page 24.
- Our simulator can solve problems of surface analyses for metals and semiconductors, chemical reactions of catalysts, and observations of DNA and bio-related materials.→Please look at the page 28.
- You can expect to use our simulator for industrial production of nanoscale devices in future.→Look at the page 29.
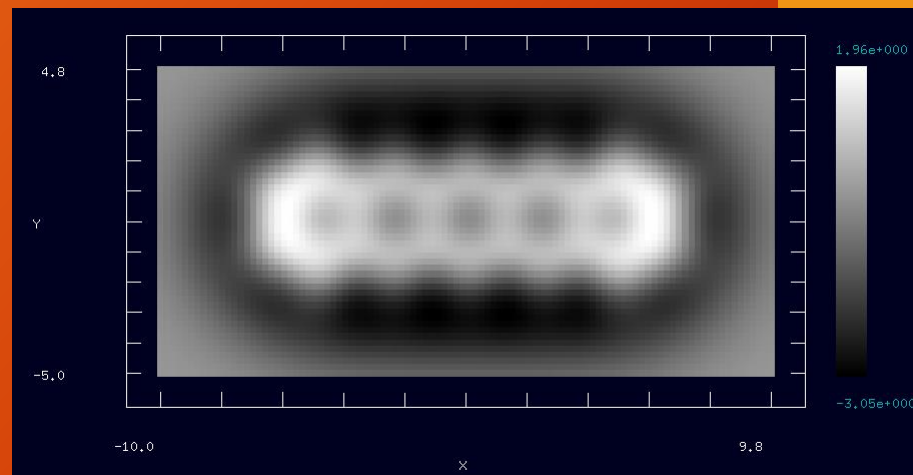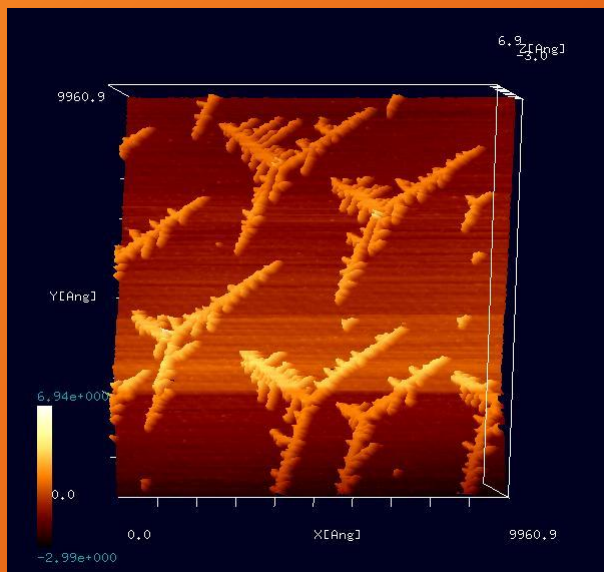
An effective presentation of experimental image data
[Offered by the Fukutani laboratory in Institute of Industrial Science, the University of Tokyo. (The two-dimensional self-organized fractal islands of Au grown on the Ir crystal by annealing.) S. Ogura et al., Phys. Rev. B **73**, 125442 (2006); S. Ogura and K. Fukutani, J. Phys.: Condens. Matter **21** (2009) 474210.]

The AFM frequency shift image of pentacene obtained by Geometry Optimizing AFM Image simulator

Realization of simple and effective numerical simulations for experimental researchers:

By using the excellent graphical user interface, experimental researchers can perform various simulations of the Scanning Probe Microscope.
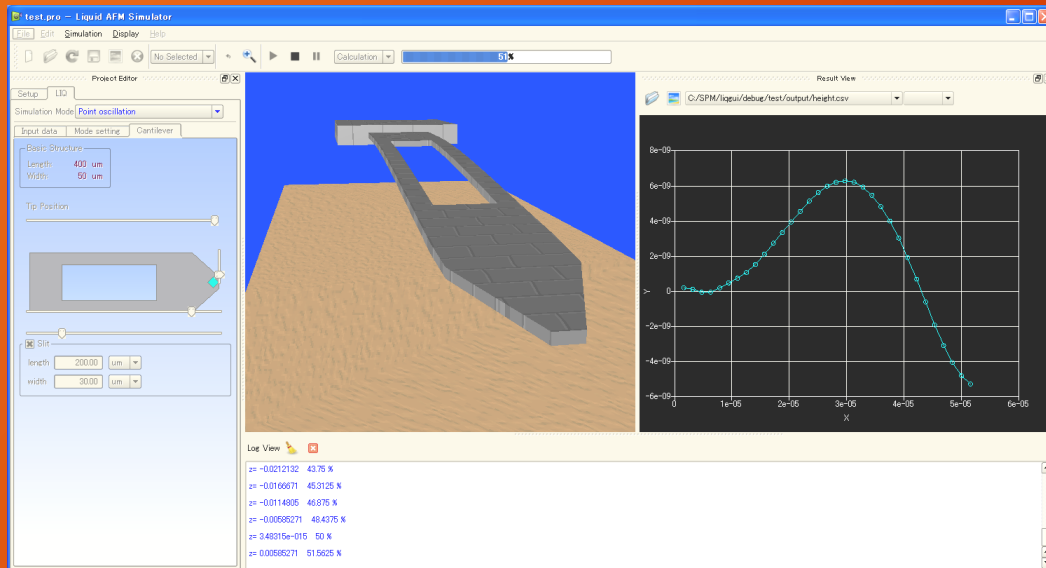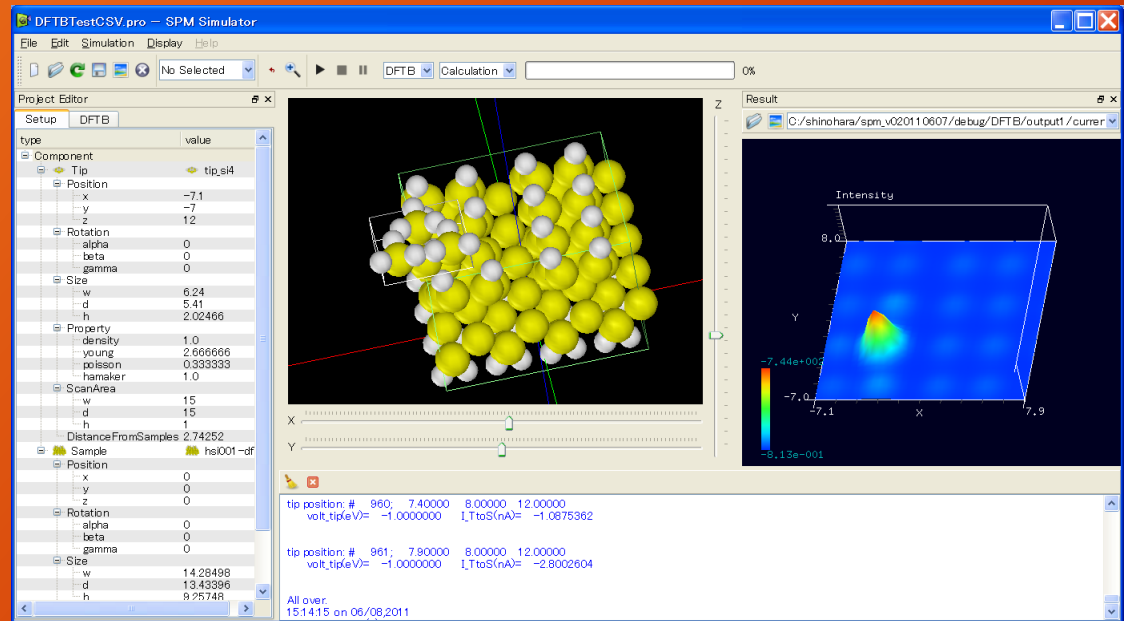
An example of performance with the Graphical User Interface

➡ Accessible and instructive tools for beginners

The execution screen for simulation of the AFM cantilever in the liquid environment

The SPM simulator

Analyzer | The Experimental Image Data Processor
- The blind tip reconstruction Method
- A function to import experimental binary data in various formats

The Analyzer can extract novel knowledge by comparing both experimental data and simulation data.

GeoAFM | The Geometrical Mutual AFM simulator | The geometry
- Nanoscale devices
- Polymers and bio-related materials

Because the GeoAFM carries out simulations in a few seconds, you can use it with performing experiments simultaneously.

FemAFM | The Finite Element Method AFM simulator | The classical theory
- Nanoscale devices
- Polymers and bio-related materials

Using the FemAFM, you can simulate the viscoelastic mechanics for polymers and bio-related materials.
Generating the finite element meshes for the tip and the sample, you can simulate frequency shift AFM images by the FemAFM.

LiqAFM   The Soft Material Liquid AFM simulator   The classical theory   Polymers and bio-related materials

The LiqAFM can simulate motion of the AFM cantilever with a complex shape in the liquid environment.
The LiqAFM can simulate viscoelastic mechanics.

CG   The Geometry Optimizing AFM Image simulator   The classical theory

- Organic molecules
- Inorganic materials

The CG can simulate frequency shift AFM images.

MD   The Molecular Dynamics AFM Image simulator   The classical theory

- Organic molecules
- Inorganic materials

The MD can evaluate a force curve between the tip and the sample.

DFTB   The Quantum Mechanical SPM simulator   The quantum theory   Frequency shift AFM images for atoms and molecules, STM images, KPFM images

The DFTB realizes STM simulation with the density functional method for various kinds of atoms easily.
The DFTB is the simplest simulator that utilizes density functional method on the market.

SetModel   The SetModel generates input data for a thin layer of the semiconductor with ease.
You can construct input data for structure of the sample with various kinds of atoms freely.

An example of simulation of a frequency shift AFM image with the DFTB solver:
A hydrogen-terminated silicon tip is scanning a hydrogen-terminated silicon surface.
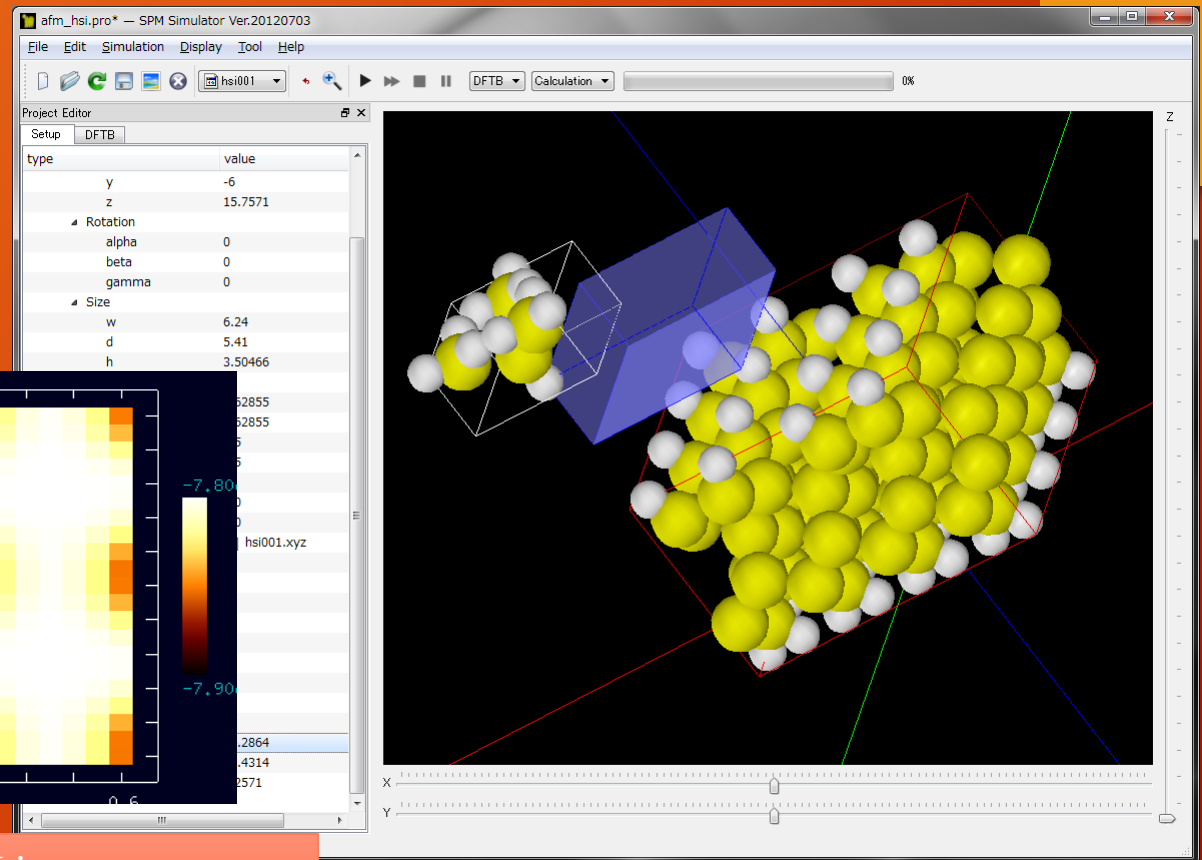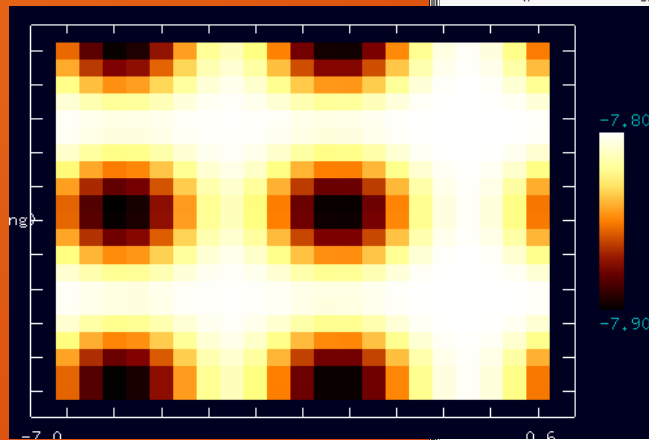
An obtained frequency shift AFM image:
Hydrogen atoms are represented as black points.

The world of the SPM simulator
Target audiences of our simulator are researchers in the field of the surface science.

Do you want to perform digital processing on experimental SPM images?
Why not try the Analyzer?
- The operational navigation system for the SPM simulator
- Explanations of functions of the Analyzer
- Introductions of functions (various input data, links to reference Web pages.
- In the reference Web pages, you can find movies that explain how to use the simulator.)
   - Estimation of the shape of tip and removal of artifacts from the experimental image
   - Digital image processing (Fourier analysis, adjustment of the contrast, etc)

Do you want to simulate AFM images of polymers and bio-related materials?
Why not try the FemAFM?
- The operational navigation system for the SPM simulator
- Explanations of functions of the FemAFM
- Introductions of functions (various input data, links to reference Web pages.
- In the reference Web pages, you can find movies that explain how to use the simulator.)
   - Simulation of the AFM for polymers (non-contact mode)
   - Simulation of the frequency shift AFM images for polymers
   - Analyses of the viscoelastic mechanics for polymers

Do you want to simulate the AFM in the liquid environment?
Why not try the LiqAFM?

The operational navigation system for the SPM simulator

Explanations of functions of the LiqAFM

Introductions of functions (various input data, links to reference Web pages.

In the reference Web pages, you can find movies that explain how to use the simulator.)

Analyses of motion of the cantilever in the liquid environment

Numerical analyses of resonant frequency of the cantilever oscillation

Analyses of viscoelastic mechanics of polymers in the liquid environment

Do you want to simulate AFM images of large polymers rapidly?
Why not try the GeoAFM?

The operational navigation system for the SPM simulator

Explanations of functions of the GeoAFM

Introductions of functions (various input data, links to reference Web pages.

In the reference Web pages, you can find movies that explain how to use the simulator.)

Derivation of the AFM image from shapes of the tip and the sample

Derivation of the shape of the sample from the AFM image and the shape of the tip

Derivation of the shape of the tip from the AFM image and the shape of the sample

Do you want to simulate the AFM for organic molecules of the order of an angstrom with the classical theory?

Why not try the CG?

The operational navigation system for the SPM simulator

Explanations of functions of the CG

Introductions of functions (various input data, links to reference Web pages.
In the reference Web pages, you can find movies that explain how to use the simulator.)

Simulation of the two-dimensional map of the force with constant height mode

Simulation of the AFM image with contact mode

Simulation of the frequency shift AFM image

Simulation of the force curve

Simulation of the AFM image with minimum force mode

Do you want to simulate the AFM for organic molecules of the order of an angstrom with the classical theory in the liquid environment?

Why not try the CG-RISM?

The operational navigation system for the SPM simulator

Explanations of functions of the CG-RISM

Introductions of functions (various input data, links to reference Web pages.
In the reference Web pages, you can find movies that explain how to use the simulator.)

Simulation of the two-dimensional map of the force with constant height mode

Simulation of the force curve

Simulation of the frequency shift AFM image

Do you want to simulate the AFM for organic molecules of the order of an angstrom with the molecular dynamics theory?

Why not try the MD?

The operational navigation system for the SPM simulator

Explanations of functions of the MD

Introductions of functions (various input data, links to reference Web pages.

In the reference Web pages, you can find movies that explain how to use the simulator.)

Simulation of the force curve

Simulation of the two-dimensional map of the force with constant height mode

Simulation of the frequency shift AFM image

Simulation of the relaxation of the structure of the molecule

The world of the SPM simulator

Our simulator can solve problems of surface analyses for metal and semiconductor, chemical reactions of catalyst, and observations of DNA and bio-related materials.

Do you want to simulate the STM, the AFM, and the KPFM for inorganic materials, semiconductors, and metals of the order of an angstrom with the quantum mechanics?
Why not try the DFTB?

The operational navigation system for the SPM simulator

Explanations of functions of the DFTB

Introductions of functions (various input data, links to reference Web pages.

In the reference Web pages, you can find movies that explain how to use the simulator.)

Simulation of the frequency shift AFM image

Simulation of the image of the tunneling current with constant height mode

Simulation of the image of the STM topography with constant tunneling current

Simulation of the KPFM image

Do you want to generate input data of crystal structures for inorganic materials, semiconductors, metals, and carbon nanotubes?
Why not try the SetModel?

The operational navigation system for the SPM simulator

Explanations of functions of the SetModel

The world of the SPM simulator
You can expect to use our simulator for industrial production of nanoscale devices in future.

How to use the SPM simulator is explained in the following pages for each industrial sector.

The chemical industry, the biology industry, the food industry, the healthcare industry (cosmetic products, soaps and detergents, pharmacy products)

    Simulation of observation of single polymers by the SPM simulator

        Documents

        Case examples

    Simulation of observation of polymers in the liquid environment by the SPM simulator

        Documents

        Case examples

    Simulation of observation of bio-related materials by the SPM simulator

        Documents

        Case examples

The textile fabric industry
   Simulation of observation of microstructures of fabric by the SPM simulator
      Documents
      Case examples

The semiconductor industry, the electronics industry, the steel industry (organic semiconductors, inorganic semiconductors, metals)
   Simulation of observation of organic semiconductors by the SPM simulator
      Documents
      Case examples
   Simulation of observation of inorganic semiconductors and metals by the SPM simulator
      Documents
      Case examples

The automotive industry, the chemical industry (exhaust gas catalysts, catalysts for chemical reactions)

Simulation of observation of catalysts by the SPM simulator

Documents

Case examples

The electronics industry (displays, lithium ion batteries)

Simulation of observation of lithium ion batteries and transparent electrodes by the SPM simulator

Documents

Case examples

A program of the web seminar (part 0)

You can learn how to use the SPM simulator with a tutorial and free trial use of the software.

For a beginner of the SPM simulator, we prepare a tutorial and a plan for refining the software in future.

https://www.aasri.jp/pub/spm/pdf/spm_tutorial_design.pdf

http://www.aasri.jp/pub/spm/pdf/spm_further_improving_plan_20121004.pdf

We provide customized software package for you.

https://www.aasri.jp/pub/spm/pdf/catalog/kakaku_uc.pdf#page=31

We prepare introductory web pages for beginners of the SPM simulator.

Visiting these web pages, you can learn how to use the software.
https://www.aasri.jp/pub/spm/assistant/SPM_Simulator_assistant_top.htm

Going ahead with web pages according to an instruction given in each page, you can automatically reach an optimum solver which is suitable for your own problem.

You can find a typical example resembling a simulation that you want to perform.

Visiting a web page for editing a project file, you can obtain an input data file for your own simulation with rewriting a few parameters of physical quantities.

Thus, you can edit an input data file with ease.

What you have to do is just downloading the project file generated automatically from the web page.

Letting the SPM simulator read the input data file that you have downloaded, you can start the simulation just by clicking the start button.

If you have any questions, please consult us by e-mail.

spm-simulator-howto@aas-ri.co.jp

An abstract of the web seminar
A basic course for simulations of the AFM

Exercises of simulations of AFM for organic and bio-related molecules

Fields: bio-related materials, polymers, organic semiconductors

Contents of exercises:

Exercises for basic operations of simulations

Exercises for how to use the GUI of the simulator

Exercises for performing simulations with actual examples

To apply for the web seminar, please feel free to send an e-mail to us:

spm-simulator-howto@aas-ri.co.jp

A program of the web seminar (part 1)

[1] Exercises: basic operations for simulations

Operation of the software (Chapter 2 in the tutorial)

A program of the web seminar (part 2)

[2]Exercises for using the GUI of the simulator

Case studies in the tutorial (Chapter 3 in the tutorial)

1. Geometrical Mutual AFM Simulator

Simulation of the AFM image, from the data of the tip and the sample
Glycoprotein (1clg) on HOPG using a quadrilateral pyramid probe tip
[GeoAFM_CalcImage_Polymer_002a]
An explanation in a PowerPoint file (pptx format, 244.9 KB)
A project file (zip format, 50.4 KB)
A reference in the web page
Simulation of the sample surface, from the tip data and the observed AFM image
Removing artifacts caused by a broken double tip from the AFM image of Glycoprotein (1clg) on HOPG
[GeoAFM_CalcSample_Polymer_002]
An explanation in a PowerPoint file (pptx format, 201.6 KB)
A project file (zip format, 19.3 KB)
A reference in the web page
Simulation of the tip surface, from the sample data and the observed AFM image
Using the AFM image of Glycoprotein (1clg) on HOPG and structural data of the sample
[GeoAFM_CalcTip_Polymer_001]
An explanation in a PowerPoint file (pptx format, 196.0 KB)
A project file (zip format, 58.0 KB)
A reference in the web page

A program of the web seminar (part 2)

[2]Exercises for using the GUI of the simulator

Case studiesin the tutorial (Chapter 3 in the tutorial)

2. Finite Element Method AFM Simulator   Simulation of an AFM image of an organic macromolecule (non-contact mode)
                                                Simulation of an AFM frequency shift image of a crystalline silicon surface (frequency shift image mode)
                                                Simulation of an AFM viscoelastic dynamics analysis of a crystalline silicon surface (viscoelastic dynamics mode)

3. Soft Material Liquid AFM Simulator   Motion of the cantilever in water
                                                Frequency spectrum of the cantilever
                                                Cantilevers having complex shapes
                                                Simulation with viscoelastic dynamics

4. Classical Force Field AFM Simulator   Example of calculating the frequency shift image of pentacene in vacuum
                                                Example of calculating force curve in aquatic environment
                                                Example of calculating force curve of chain alkane

5. Quantum Mechanical SPM Simulator   Example of AFM (frequency shift) image simulation
                                                Examples of STM simulation   (1) Simulation for a tunneling current image
                                                                               (2) Calculation of Scanning Tunneling Spectroscopy
                                                Simulation for a KPFM simulation
                                                Band calculation

6. Movies for examples of calculation
A simulation of tunneling current in a plate of Au(111) for STM (constant height mode) with the DFTB solver

A program of the web seminar (part 3)

[3]Exercises for using the GUI of the simulator

Image Comparison in the tutorial (Chapter 4 in the tutorial)

A program of the web seminar (part 4)

[4]Exercises for using the GUI of the simulator

Sample Modeling in the tutorial **(Chapter 5 in the tutorial)**

A program of the web seminar (part 5)

[5] Exercises for Analyzer

Digital processing of experimental data of the SPM (the tutorial)

Exercises for loading experimental binary data generated by various companies' SPM systems (the tutorial)

Loading the data, adjusting the tilt of the plate, and showing the image in perspective (case studies)

[Analyzer_ImageProcessing_009]

An explanation in a PowerPoint file (pptx format, 969.4 KB)

Experimental image data (a) (zip format, 305.6 KB)

Experimental image data (b) (SM4 format, 4.3 MB)

Experimental image data (c) (STP format, 3.0 MB)

Experimental image data (d) (STP format, 3.0 MB)

Experimental image data (e) (ibw format, 336.2 KB)

Experimental image data (f) (zip format, 129.5 KB)

Experimental image data (g) (zip format, 151.4 KB)

Experimental image data (h) (zip format, 166.6 KB)

A reference in the web page (1)

A reference in the web page (2)

A reference in the web page (3)

A reference in the web page (4)

A reference in the web page (5)

A reference in the web page (6)

A reference in the web page (7)

A program of the web seminar (part 6)

[6] Exercises for Analyzer

Digital processing of experimental data of the SPM **(the tutorial)**

An exercise for estimation of the tip shape (the tutorial)

Estimation of the tip shape / Removal of the tip-shape influence (the case studies)

[Analyzer_TipEstimation_001]

An explanation in a PowerPoint file (pptx format, 259.9 KB)

An AFM image of artificial objects obtaine by a broken double tip (cube format, 1.5 MB)

A reference in the web page

A program of the web seminar (part 7)

[7] Exercises for Analyzer

Digital processing of experimental data of the SPM **(the tutorial)**

Exercises of Fourier analyses and high-resolutionizing of images **(the tutorial)**

[Analyzer_ImageProcessing_003]
An explanation in a PowerPoint file (pptx format, 438.5 KB)
Experimental image data (a) (cube format, 6.0 MB)
Image data generated with high-frequency emphasis filter (a) (cube format, 6.0 MB)
Image data generated with low-frequency emphasis filter (a) (cube format, 6.0 MB)
Experimental image data (b) (cube format, 6.0 MB)
Image data generated with high-frequency emphasis filter (b) (cube format, 2.7 MB)
Image data generated with low-frequency emphasis filter (b) (cube format, 2.9 MB)
A reference in the web page (1)
A reference in the web page (2)

An exercise of contrast adjustment for experimental image data **(the tutorial)**

[Analyzer_ImageProcessing_006]
An explanation in a PowerPoint file (pptx format, 283.0 KB)
Experimental image data (cube format, 6.0 MB)
Image data whose contrast is adjusted (cube format, 6.0 MB)
A reference in the web page

A program of the web seminar (part 8)

[8] Exercises for GeoAFM and Analyzer
Rapid simulations for AFM images of polymers
Exercises of geometrical mutual AFM simulation for experimental data of the sample, theoretical data of the sample, and structural data of the tip (the tutorial)
Calculation of the AFM image from the structural data of the sample and the tip
  GeoAFM (Geometrical mutual AFM simulator) CalcImage (the case studies)
Calculations of the structure of the sample from the AFM image and the structural data of the tip
  GeoAFM (Geometrical mutual AFM simulator) CalcSample (the case studies)
Calculation of the structure of the tip from the AFM image and the structural data of the sample
  GeoAFM (Geometrical mutual AFM simulator) CalcTip (the case studies)

Please learn how to use the simulators from practical exercises.

Removal of artifacts caused by a broken double tip from the experimental AFM image (the tutorial)
[Analyzer_TipEstimation_002]
An explanation in a PowerPoint file (pptx format, 255.6 KB)
Experimental image data of STM (cube format, 1.5 MB)
Estimated structural data of the tip (cube format, 4.0 KB)
An image of the STM whose artifacts are removed (cube format, 640.1 KB)
A reference in the web page

A program of the web seminar (part 9)

[9] Exercises for FemAFM (Finite Element Method AFM simulator)
A simulation for AFM with considering deformation of a polymer **(the tutorial)**
An exercise of a simulation of the AFM image with non-contact mode (the tutorial)
Calculation of the two-dimensional map of forces with non-contact mode
FemAFM ConstHeight (the case studies)
An exercise of a simulation for an AFM frequency shift image (the tutorial)
AFM frequency shift images FemAFM FreqShift (the case studies)
An exercise of an AFM viscoelastic dynamics analysis (the tutorial)
Analyses of viscoelastic contact problems FemAFM Viscoelastic (the case studies)

Please learn how to use the simulator with practical examples.

A program of the web seminar (part 10)

[10] Exercise for LiqAFM (Soft Material Liquid AFM simulator) (the tutorial)
Oscillation of the cantilever: BarMotion [Point oscillation] (the case studies)
Resonance curves: Resonance [Parameter Scan] (the case studies)
Viscoelastic contact problems: Viscoelastic [Point oscillation] (the case studies)

Please learn how to use the simulator with practical examples.

A program of the web seminar (part 11)

[11] Exercises for CG-RISM (Atomic-scale simulation of the AFM in liquid environment) (the tutorial)

A two-dimensional map of forces with constant-height mode: [ConstZ] (the case studies)

Force curves: [ForceCurve] (the case studies)

AFM frequency shift images: [ncAFM-ConstZ] (the case studies)

Please learn how to use the simulator with practical examples.

A program of the web seminar (part 12)

[12-1] An exercise for FemAFM_DLVO
Functions according to the DLVO theory in the Finite Element Method AFM simulator (the tutorial)

[12-2] An exercise for macroKPFM_DLVO
Functions according to the DLVO theory in the macroKPFM simulator (the tutorial)

Please learn how to use the simulator with practical examples.