Scanning Probe Microscope Simulator

ver.β

Reference Manual

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Introduction

This document is a reference manual of the scanning probe microscopy (SPM) simulator. Details of all parameters and initial settings are descibed for the five simulators that are "Geometrical Mutual simulator" (GEO), "Finite Element Method AFM simulator" (FEM), "Soft Material Liquid AFM Simulator" (LIQ), "Classical Force Field AFM simulator" (CG/MD), and "Quantum Mechanical SPM Simulator" (DFTB). We hope that the document is useful and helpful for your working.

1. Geometrical Mutual AFM simulator

Outline

Geometrical Mutual AFM simulator (GeoAFM) provides users with a kind of a three-way data processor. Among three geometrical elements, a tip, sample material and its AFM image, this module reconstructs the one out of the other two. For example, it can reconstruct the AFM image from information about shapes of the tip and the sample material. The GeoAFM accomplishes the calculation very rapidly, and it takes only a few seconds.

Throughout the simulation, the GeoAFM assumes that the tip always touches the surface of the sample material, so that it scans the surface of the sample in the so-called contact mode.

In the following paragraphs, we look around parameters that we have to supply to the GeoAFM for carrying out simulations actually.

Configuration of parameters for the GeoAFM

As mentioned above, the GeoAFM works as a kind of the three-way data processor, so that we can use it in the following three manners:

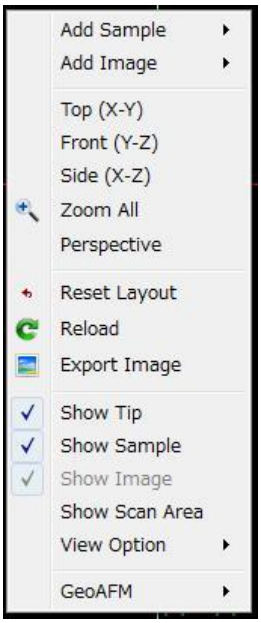
1. Obtaining the AFM image form the geometrical data of the tip and the surface of the sample material
2. Obtaining the geometry of the surface of the sample material from the geometrical data of the tip and the AFM image observed
3. Obtaining the geometry of the tip from the geometrical data of the surface of the sample material and the AFM image observed

Before performing one of the above three simulations, you have to load the following two data files through the item [Project Editor] > [Setup] > [Component] in each case:

1. [Tip] and [Sample]
2. [Tip] and [Image]
3. [Sample] and [Image]

To carry out the numerical simulation with the GeoAFM, you have to load the above two data files. Then, putting the cursor on the main window, where images of the data files are

displayed, and right-clicking on it, you will obtain the context menu shown on the right.



Here, the item [GeoAFM], which is located at the bottom of the context menu, is important for us. Putting the cursor on this item, you can select the following three items:

- [Show Simulated Image]
- [Set GeoAFM Resolution]
- [Export Simulated Data]

Functions of the above three items are as follows:

[Show Simulated Image]

Choosing this item, you can display an output image fed by the GeoAFM in the main window.

If you want to delete the other two images, which are supplied as input data to the GeoAFM, remove ticks of the two corresponding items out of [Show Tip], [Show Sample] and [Show Image] in the context menu.

[Set GeoAFM Resolution]

Choosing this item, you can define a resolution of a geometrical object, which we are going to obtain with the numerical simulation. A unit of the resolution is given by angstrom and you can adjust its value by 0.1. The minimum and maximum values of the resolution are given by 0.1 [angstrom] and 10.0 [angstrom], respectively. A default value of the resolution is put at 5.0 [angstrom] previously.

[Export Simulated Data]

Choosing this item, you can store up the image obtained by the numerical calculations as a data file, which is reusable for other purposes later. This item is effective only if the above item [Show Simulated Image] is turned on. The numerical data is saved as the “cube” file. The extension “.cube” stands for the SPM simulators’ own file format.

2. Finite Element Method AFM simulator

Outline

Finite Element Method AFM simulator (FemAFM) derives an AFM image from the geometrical data and physical properties of a tip and sample material. The van der Waals interaction between a tip and a sample material is taken into account in case of the non-contact mode. On the other hand, the adhesion forces due to the JKR (Johnson, Kendall, Roberts) theory are considered in case of the contact mode. The FemAFM solves the differential equation of elasticity with the finite element method.

The FemAFM assumes that each of the sample and the tip at the top of a cantilever consists of a uniform continuous elastic body. Therefore, the microscopic structures of atoms/molecules in the tip/sample are not taken into consideration at all. The FemAFM is better suited to simulate AFM images of surface structures of a few hundred angstroms.

The FemAFM treats three calculation modes as below.

- [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.
- [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.
- [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.

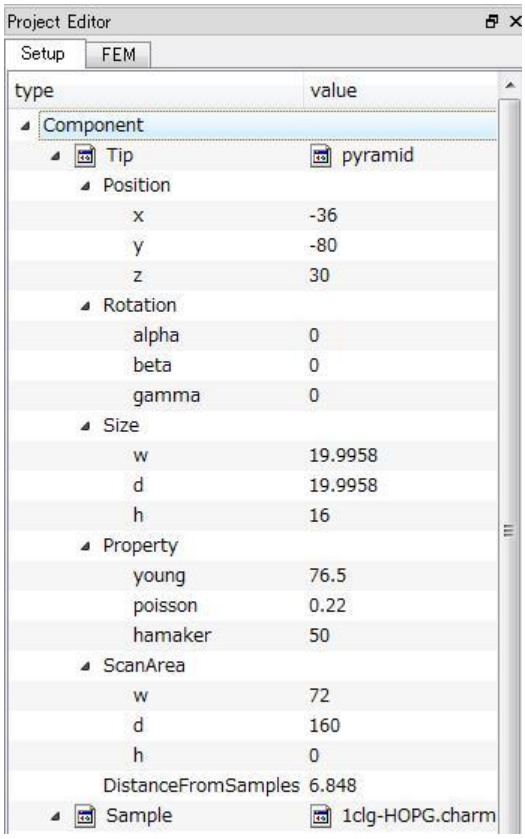
In the following paragraphs, we look around parameters that we have to supply to the FemAFM for carrying out simulations actually.

Configuration of parameters for the FemAFM

Before performing simulations of the FemAFM, you have to load the two data files, [Tip]

and [Sample], through the item [Project Editor] > [Setup] > [Component]. For each of these data, [Tip] and [Sample], you can put some parameters as explained in the following paragraphs.

First, we can put parameters for [Tip] as follows:



Parameters [x], [y] and [z] of [Position] represent the initial coordinates of the tip. The unit of the coordinate is given by angstrom. The origin of the three-dimensional Cartesian coordinate system is put at the center of a substrate where the sample material lies. (Thus, the sample material lies on the xy plane.) From the point given by [Position], the tip starts scanning.

Parameters [alpha], [beta] and [gamma] of [Rotation] represent the angles of clock-wise rotations about x, y and z axes, respectively. The Cartesian system of the axes (x, y and z) is fixed on the tip. The unit of angle is given by a degree, so that one complete turn is equal to 360 degrees.

Parameters [w], [d] and [h] of [Size] represent width, depth and height of whole of the tip, respectively. Directions of the dimensions, [w], [d] and [h] are taken along the Cartesian coordinates, x, y and z, respectively.

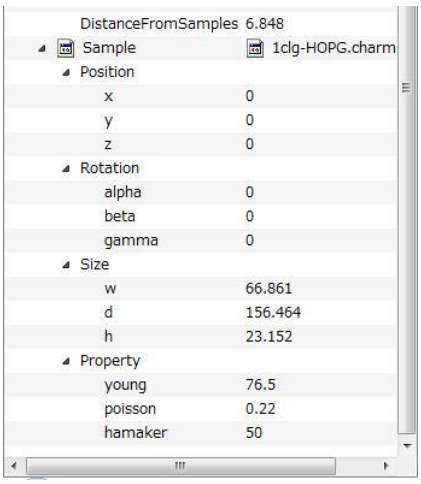
Parameters of [young], [poisson] and [hamaker] of [Property] represent Young's modulus, Poisson's ratio and the Hamaker constant for the tip, respectively. The unit of the Young's modulus is given by [GN/m2], where "G" stands for ten to the ninth power. The unit of the Hamaker constant is given by [zJ], where "z" stands for the inverse of ten to the twenty-first power. In the following list, we describe these parameters for typical material.

Material	Young's modulus [GN/m^2]	Poisson's ratio	Hamaker constant [zJ]
SiO_2	76.5-97.2	0.22	50-60
Al_2O_3	250-350	0.24	110-150
Si_3N_4	320	0.29	140-220
Au	78	0.44	300-400
Ag	82.7	0.367	400-500
Cu	129.8	0.343	300-400

Parameters [w], [d] and [h] of [Scan Area] represent rectangular region where the tip scans. The unit of [w], [d] and [h] is given by angstrom. Because this [Scan Area] lies on the xy plane, the value of [h] has to be equal to zero. From the starting point given by [Position] above, the tip scans this rectangular area.

Parameter [DistanceFromSamples] represents the minimum distance between the tip and the surface of the sample material. Its unit is given by angstrom.

Second, we can put parameters for [Sample] as follows:



Parameters [x], [y] and [z] of [Position] are used for moving the sample material at the beginning of the simulation. The unit of them is given by angstrom. These parameters, [x], [y] and [z], represent a three-dimensional vector, whose initial point is the origin of the

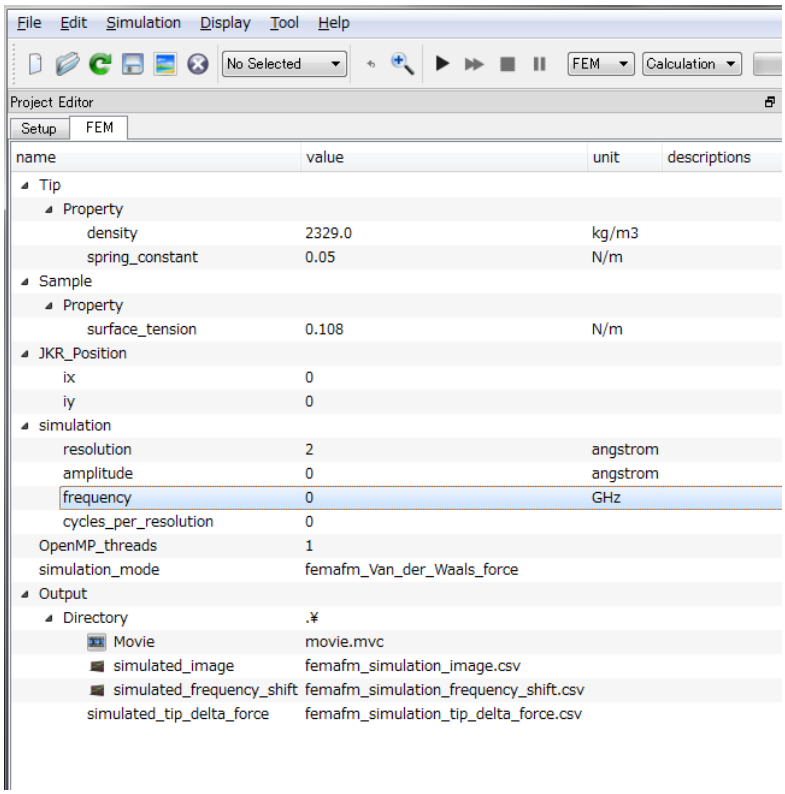
Cartesian coordinate system. The origin is put at the center of a substrate where the sample material lies. (Thus, the sample material lies on the xy plane.) The sample material is moved along this vector. These parameters are convenient when you want to adjust the height of the sample material, which lies on a substrate, for example.

Parameters [alpha], [beta] and [gamma] of [Rotation] represent the angles of clock-wise rotations about x, y and z axes, respectively. The Cartesian system of the axes (x, y and z) is fixed on the center of the substrate, where the sample material is lying. The unit of angle is given by a degree, so that one complete turn is equal to 360 degrees.

Parameters [w], [d] and [h] of [Size] represent width, depth and height of whole of the sample, respectively. Directions of the dimensions, [w], [d] and [h] are taken along the Cartesian coordinates, x, y and z, respectively.

Parameters, [young], [poisson] and [hamaker] of [Property], represent Young's modulus, Poisson's ratio and the Hamaker constant for the sample material, respectively. The unit of the Young's modulus is given by [GN/m^2], where "G" stands for ten to the ninth power. The unit of the Hamaker constant is given by [zJ], where "z" stands for the inverse of ten to the twenty-first power.

Moreover, in the tab [Project Editor] > [FEM], we can adjust the following parameters.



name	value	unit	descriptions
Tip			
Property			
density	2329.0	kg/m3	
spring_constant	0.05	N/m	
Sample			
Property			
surface_tension	0.108	N/m	
JKR_Position			
ix	0		
iy	0		
simulation			
resolution	2	angstrom	
amplitude	0	angstrom	
frequency	0	GHz	
cycles_per_resolution	0		
OpenMP_threads	1		
simulation_mode	femafm_Van_der_Waals_force		
Output			
Directory	.¥		
Movie	movie.mvc		
simulated_image	femafm_simulation_image.csv		
simulated_frequency_shift	femafm_simulation_frequency_shift.csv		
simulated_tip_delta_force	femafm_simulation_tip_delta_force.csv		

Beneath the [Property] of the [Tip], we adjust the density of the tip material as [density] and the spring constants of the cantilever as [sprint_constant].

Beneath the [Property] of the [Sample], we adjust the surface tension of the sample as [surface_tension].

Those three parameters, [Tip] → [density], [Tip] → [spring_constant] and [Sample] → [surface_tension], are required to describe the JKR theory, and therefore used in the [frequency shift image mode] and the [viscoelastic dynamics mode].

Parameters [ix] and [iy] of [JKR_Position] are used in the [viscoelastic dynamics mode]. [ix] and [iy] are the running numbers along x- and y-direction of divided meshes in the scanning area. [ix] and [iy] start from 1 from the bottom left corner. The [viscoelastic dynamics mode] simulation is performed at the specified point on the xy-plane.

On the item [simulation], we can adjust the following three parameters:

- [resolution]: This parameter defines the resolution for the simulation of the FemAFM. The resolution represents the minimum length of the numerical calculations for obtaining the AFM image. To be precise, the resolution represents a typical length between neighboring vertices of a mesh, which is prepared for numerical calculations of the finite element method. A unit of the resolution is given by angstrom and you can adjust its value by 0.1. The maximum value of the resolution is given by 10.0, and its default value is put at 2.0 [angstrom] previously.
- [amplitude]: This parameter defines the maximum amplitude of an oscillation of the cantilever. While the tip scans the surface of the sample material, the cantilever oscillates in the direction of the z axis.
- [cycles_per_resolution]: This parameter defines the period of the oscillation of the cantilever. While the tip scans the surface of the sample material, the cantilever oscillates in the direction of the z axis.

The [amplitude] and the [cycles_per_resolution] are used in the [frequency shift image mode] and in the [viscoelastic dynamics mode].

The parameter [OpenMP_threads] means the number of CPUs for the parallel computing.

The parameter [simulation_mode] switches the three simulation modes.

- Select [femafm_Van_der_Waals_force] for the [Non-contact mode] simulation.
- Select [femafm_frequency_shift] for the [frequency shift image mode] simulation.

- Select [femafm_JKR] for the [viscoelastic dynamics mode] simulation.

On the item [Directory] beneath [Output], a path “¥.” is put as the default. This implies that data files obtained as results of numerical simulations are put in the folder of the current project, where the present project file is stored up.

Beneath the [Directory], there are several file names as follows.

- “movie.mvc” is a video file, which records sequential movements of the tip scanning on the surface of the sample material.
- “femafm_simulation_image.csv” is a data file of the AFM image obtained with numerical simulation by the [Non-contact mode].
- “femafm_simulation_frequency_shift.csv” is a data file of the frequency shift AFM image obtained with numerical simulation by the [frequency shift image mode].
- “femafm_simulation_tip_delta_force.csv” is a data file of the tip displacement and the external force to the tip as a function of time obtained with numerical simulation by the [viscoelastic dynamics mode].

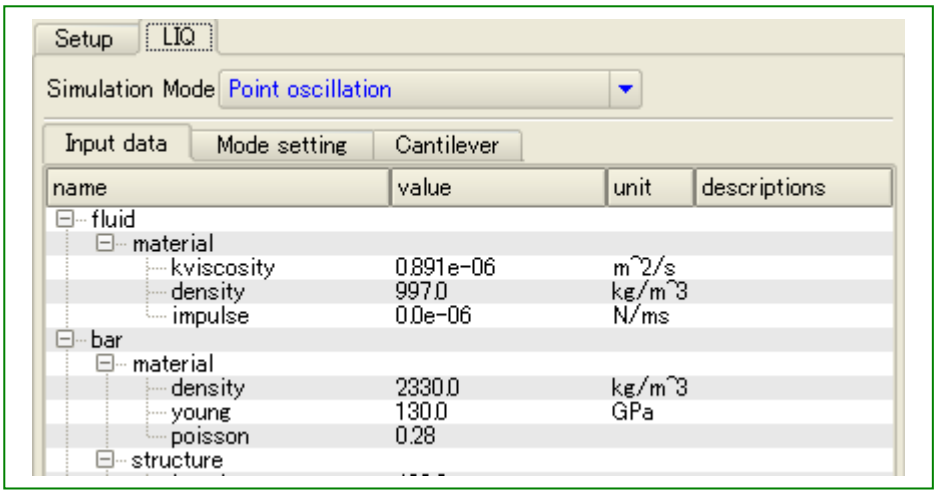
3. Soft Material Liquid AFM Simulator

Introduction

“Soft Material Liquid AFM Simulator” calculates bending and twisting oscillation of an elastic cantilever, embedded in liquid, tapping its tip on soft material samples. This software calculates both the elastic dynamics of the cantilever and fluid dynamics around the cantilever simultaneously. Many aspects of cantilever motion in liquid can be estimated by this software. For example, the resonance frequency of the cantilever designed to work in vacuum, and how it changes in liquid, or by tapping soft material samples.
The following is explanation of initial setting parameter for this simulator.

Input Parameters

Input parameters viewer is shown as below picture.



Parameters of simulator for soft material liquid AFM in liquid has five categories.

(1) for Fluid

We here explain the parameters for fluid. The kinematic viscosity and the density of the fluid are set up. In this calculation you can also consider the impulsive force from liquid molecules.

fluid		
material		
kviscosity	0.891e-06	m^2/s
density	500.0	kg/m^3
impulse	0.0e-6	N/ms

fluid : setting for fluid

material : setting for the material properties of the fluid

kviscosity

Kinematic viscosity in [m^2/s]. Notice that this differs from the static viscosity.

density

Density in [kg/m^3].

impulse

Molecular random impulsive force per unit length and time, in [N/ms].

The kinematic viscosity and the density of water at 25 ºC are 0.891×10^{-6} [m^2/s] and 997.0 [kg/m^3], respectively. If there is no <fluid> parameter, you can simulate in vacuum.

(2) for Cantilever

In this section, we explain the material properties and the basic structure of the cantilever

bar		
material		
density	2200.0	kg/m^3
young	76.5	GPa
poisson	0.22	
friction	0.	
hamaker	5.0e-20	J

material		
density	2330.0	kg/m^3
young	130	GPa
poisson	0.28	

`bar` : setting for cantilever

`material` : setting for the material properties of the cantilever

`density`

Density in [kg/m^3].

`young`

Young's modulus in [GPa].

`poisson`

Poisson's ratio.

`friction`

Friction coefficient between the fluid and the cantilever material (dimensionless). (*)

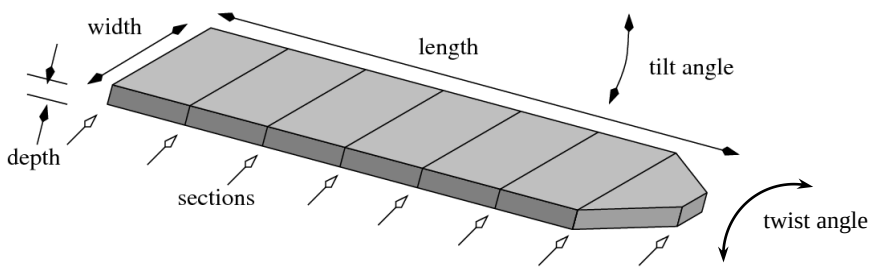
`hamaker`

Hamaker constant of the cantilever material in [J]. (*)

(*) These are used in the simulation with the viscoelastic dynamics.

A sample project file contains the parameters for a silicon cantilever; the density 2330 [kg/m^3], the Young's modulus 130 [GPa] and the Poisson's ratio 0.28.

Next, we set a structure of the cantilever and an attached probe tip. A rough picture of the cantilever is shown below.



structure		
length	400	um
width	50	um
depth	4	um
angle	0.0	deg
twist	0.0	deg
sections	17	
tip		
position	400	um
width	0.0	um
radius	25.0	nm
spotlight		
position	400	um
distance	1000.0	um
angle	0.0	deg

structure : setting for the structure of the cantilever

length

Total length in [μm].

width

Total width in [μm].

depth

Total thickness in [μm].

angle

Downward tilt angle in [degree]. Pay attention that the front edge of the cantilever does not collide to the floor.

twist

Twist angle in [degree].

sections

The number of sections of the cantilever.

tip : setting for the probe tip

position

Longitudinal position of the probe tip in [μm]. When the probe tip locates at the end of the cantilever, this value is the same as that of [structure] > [length]

width

Lateral position of the probe tip in [μm]. When the probe tip locates at center of the cantilever, input the width value “0.0”.

radius

Curvature radius of the probe tip in [nm].

spotlight : setting for the laser beam

position

Position irradiated by the laser beam. It is usually the same as the total length of the cantilever, so that the beam aims at the front edge.

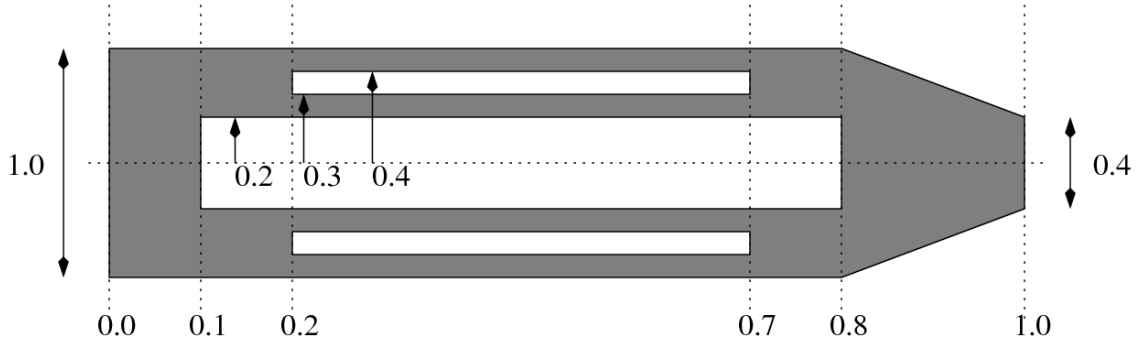
distance

Distance from the irradiated position to the detector.

angle

Incident angle of the laser beam, from the vertical axis.

We can also design a shape of the cantilever. For example, we can make a sharpened edge and make holes on the cantilever, by setting as follows.




```
<body>
  <section> 0.0 1.0 1.0 </section>
  <section> 0.8 1.0 1.0 </section>
  <section> 1.0 0.4 1.0 </section>
</body>
<split name="inside split">
  <section> 0.1 0.0 0.2 </section>
  <section> 0.8 0.0 0.2 </section>
</split>
<split name="outside split">
  <section> 0.2 0.3 0.4 </section>
  <section> 0.7 0.3 0.4 </section>
</split>
```

We specify a ratio (from 0.0 to 1.0) to mean a length or a width.

<body> : Design a shape of the cantilever by specifying several cross sections.

<section> : There are three parameters;

Ratio of a length-position along the length-direction,

Ratio of a width along the width-direction at the position,

Ratio of a thickness along the thickness-direction at the position.

<split> : Design a shape of a hole by specifying several cross sections. You can make another hole using a new <split> tag.

<section> : There are three parameters;

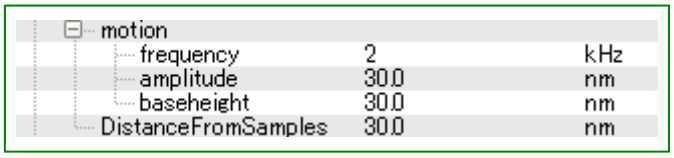
Ratio of a length-position along the length-direction,

Ratio of a starting width along the width-direction at the position,

Ratio of a last width along the thickness-direction at the position.

Finally, we explain the setting for oscillation of the cantilever. The basement of the cantilever is forced to oscillate by sin curve. The oscillation curve is written by

$$H(z=0,t) = H_o + A\sin(2\pi ft) + A_{sub}\sin(2\pi f_{sub}t)$$



motion		
frequency	2	kHz
amplitude	30.0	nm
baseheight	30.0	nm
DistanceFromSamples	30.0	nm

motion : setting for oscillation of basement of the cantilever.

frequency

Frequency f in [kHz].

amplitude

Amplitude A in [nm].

baseheight

The height from the floor to the basement of the cantilever, H_o in [μm].

subfrequency

sub-frequency f_{sub} [kHz] if there is a dual frequency excitation.

subamplitude

sub-amplitude A_{sub} [nm] if there is a dual frequency excitation.

DistanceFromSamples

Let this parameter be equal to [baseheight].

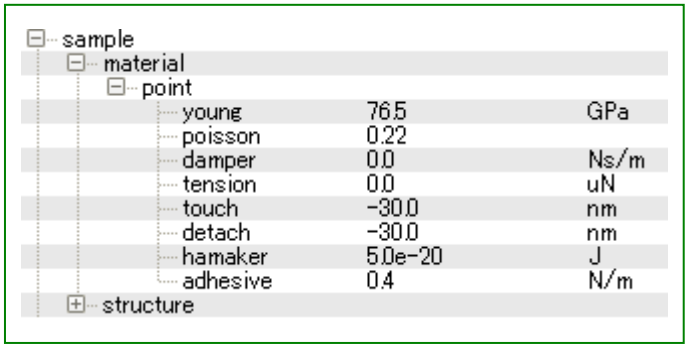
Each of these can have not only a single value but also a sequence of values, so that we can simulate a “scan” of the parameter. To do so, specify three values; the minimum value,

the maximum value and the number of scanning points, as follows.

```
<motion>
  <frequency  unit="kHz"> 5.0 15.0 11 </frequency>
  <amplitude  unit="nm"> 3.0 </amplitude>
  <amplitude  unit="nm"> 4.0 </amplitude>
  <amplitude  unit="nm"> 5.0 </amplitude>
  <baseheight unit="um"> 50.0 </baseheight>
</motion>
```

(3) for Sample

We here describe the parameters for the material properties of an elastic sample on the substrate.



sample		
material		
point		
young	76.5	GPa
poisson	0.22	
damper	0.0	Ns/m
tension	0.0	uN
touch	-30.0	nm
detach	-30.0	nm
hamaker	5.0e-20	J
adhesive	0.4	N/m
structure		

```
<structure>
  <surface>
    <section unit="um"> 0.0 0.0 </section>
    <section unit="um"> 1.0 0.0 </section>
  </surface>
</structure>
```

sample : setting for sample

structure : setting for the shape of the substrate

surface : setting for the height modulation of the macroscopic surface of the substrate, in the similar manner for making a cantilever shape.

section

There are two parameters;
Ratio of a length-position along the length-direction,
Height of the substrate at the position.

The example above assumes the flat substrate.

`material` : setting for the material properties of an elastic sample on the substrate

`point` : setting for a point contact to the sample

`young`
Young's modulus in [GPa].

`poisson`
Poisson's ratio of the elastic sample (dimensionless). (*)

`damper`
Damper coefficient in [Ns/μm].

`tension`
Tension when the probe tip makes contact with the sample, in [μN].

`touch`
Height when the tip meets the sample, measured from the initial height, in [nm].

`detach`
Height when the tip takes off from the sample, measured from the initial height, in [nm].

`hamaker`
The Hamaker constant of the sample in [J]. (*)

`adhesive`
The surface tension of the sample in [N/m]. (*)

(*) These are used in the simulation with the viscoelastic dynamics.

You can simulate without a tip on the cantilever, by setting young, poisson, damper, tension, hamaker and adhesive as zero, and setting touch and detach as the negative value of DistanceFromSamples.

There are three methods to indicate the material properties under <material> tag.

- Specify only one material property, assuming that the probe tip makes contact with the sample only at a single point.
- Specify several material properties, assuming that the probe tip makes contact with the sample at several points in sequence.
- Specify two-dimensional material properties, assuming that the probe tip makes contact with the sample by scanning on the spread sample.

In order to specify a single material property, you have to use the format below.

```
<material>
  <point>
    <spring unit="uN/nm" > 100.0 </spring>
    <damper unit="Ns/um">   0.0 </damper>
    <tension unit="uN">     0.0 </tension>
    <touch  unit="nm">     -2.5 </touch>
    <detach unit="nm">     -2.5 </detach>
  </point>
</material>
```

If you specify the other <point> tags in sequence, you can simulate at several points on the sample by turns.

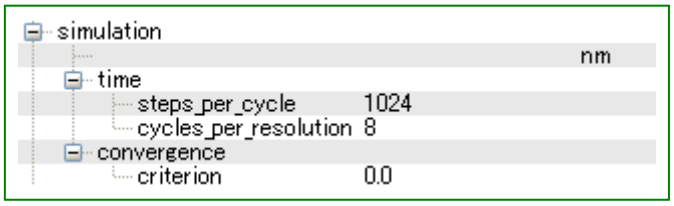
In order to specify a two-dimansional distribution of the material properties, you should prepare *.cube files which include material properties, and indicate them as follows.

```
<material>
  <field>
    <spring lengthunit="um" unit="uN/nm"> spring.cube </spring>
    <damper lengthunit="um" unit="Ns/um"> damper.cube </damper>
    <tension lengthunit="um" unit="uN"> tension.cube </tension>
    <touch lengthunit="um" unit="nm"> touch.cube </touch>
    <detach lengthunit="um" unit="nm"> detach.cube </detach>
  </field>
</material>
```

When you specify a numerical value instead of a file name, the value is uniformly applied to all scanning area.

(4) for Precision of calculation

We show the setting for a time step and convergence criteria here.



simulation : setting for the simulation

resolution : setting for the resolution

It is necessary only in case of the two-dimensional scan. You should specify the scanning resolution as follows.

```
<resolution unit="um"> 0.10 </resolution>
```

The probe tip moves along a zigzag path at even intervals of the resolution.

time : setting for a time step

steps_per_cycle

Number of time steps per one oscillation cycle. Give a large number when the calculation diverges or gets unstable.

cycles_per_resolution

Number of oscillation cycles. In case of the two-dimensional scan, it stands for the number of oscillation cycles at each resolution. In other cases, the calculation goes to the next point after the number of cycles finishes.

convergence : setting for convergence criteria

criterion

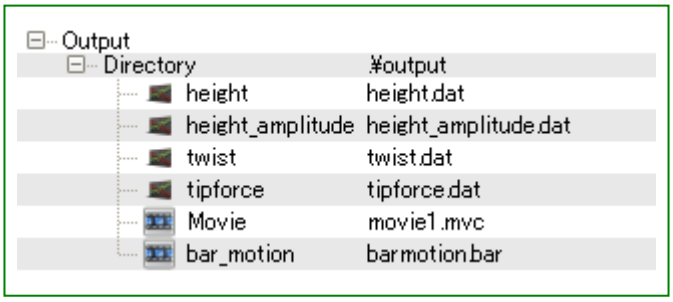
ratio of the convergence criteria whether the vibration is steady or not. The calculation will finish when

$$\frac{\left|A - A_{\mathrm{prev}}\right|}{A} \leq criterion$$

is satisfied, where A is an average amplitude during the latest cycle, while A_{prev} is that during the previous cycle. When criterion = 0.0, the convergence will not be checked, then the calculation goes on until the oscillation cycle reaches [cycles_per_resolution].

(5) for Output files

Here, the output files are set. ※At present, you are not able to change these names of files.



Output : setting for output

Directory : directory of output files.

~~**resonance_curve**~~

~~The frequency spectrum of the cantilever.~~

height

The time evolution of height at the head of a cantilever.

height_amplitude

The time evolution of height amplitude at the head of a cantilever.

twist

The twist angle of a cantilever.

`tipforce`

The time evolution of the force which the probe tip feels, when it contacts to the sample.

`delta_tipforcr`

The time evolution of distance and force between the surface of the sample and the probe tip.

`Movie`

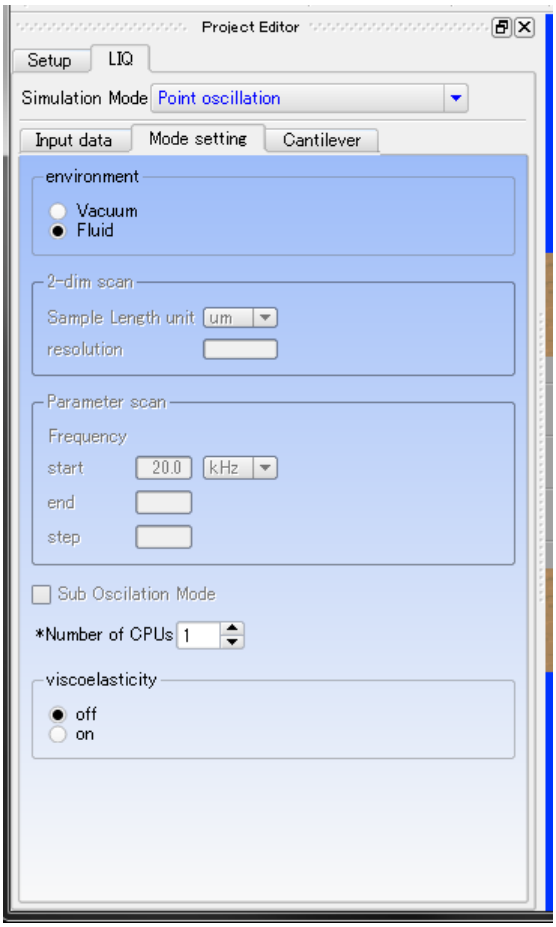
The movie of only the tip head position.

`bar_motion`

The movie of a cantilever.

(6) for other settings

We here explain [Mode setting] tab on the [LIQ] tab in the [Project Editor].



[Number of CPUs] means the number of CPUs for the parallel computing.

[viscoelasticity] switches whether the viscoelastic dynamics between the tip and the sample is taken into account or not.

4. Classical Force Field AFM Simulator

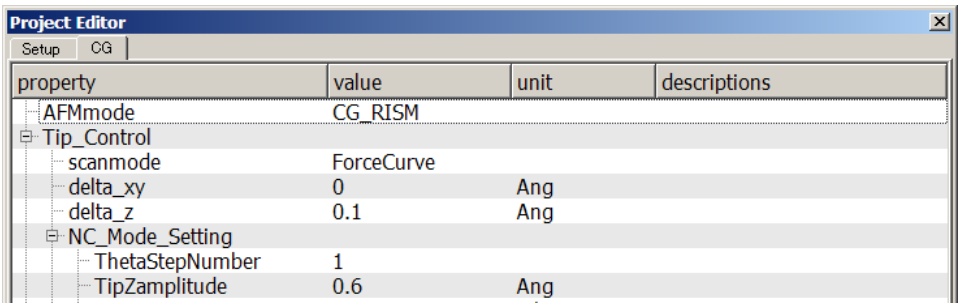
Input of the CG-AFM Simulator

In this simulator, in order to simulate the AFM image, the structural deformation of the sample molecules interacted by the scanning probe tip are calculated. Calculation procedure you operate is roughly as follows.

1. The probe tip is located at one position.
2. The structure of the sample molecules are deformed so that the energy of the system is minimized.
3. The force acting on the probe tip is calculated.
4. The probe tip is moved to the next position.
5. 2-4 are repeated.

By setting the input parameters explained below, you can control the procedure of these calculation.

For specifying the parameter of “CG-AFM Simulator”, you first select the “CG” tag of the Project Editor. This tag has four columns there.



- “property” is the name of the parameter.
- “value” is the value of the parameter.
- “unit” is the unit of the parameter.
- “descriptions” is the notes of the setting parameters.

In the following, detailed description of the meaning of each item of “property” column.

AFMmode	CG_RISM	
Tip_Control		
scanmode	ForceCurve	
delta_xy	0	Ang
delta_z	0.1	Ang
NC_Mode_Setting		
ThetaStepNumber	1	
TipZamplitude	0.6	Ang
SpringConst	200	N/m
ResoFreq	23.165	kHz
FreqShift	5	Hz
ForceConst	0.5	nN
resetStruct_atZmax	No	
OneWayForceCurve	Yes	
ForceField		

Parameter related to the whole calculation

AFMMode

Choice the calculation in either the vacuum environment or the aquatic one. When you want to choose the vacuum environment , you set ‘CG’ to this parameter. When the aquatic one, set ‘CG_RISM’.

Tip_Control : the parameters for control the probe tip.

scanmode

Scan mode of the probe tip selected from “ConstZ”, “ConstForce”, “ncAFM-ConstZ”, “ForceCurve” or “MinForceHeight”. The selected scan mode, you can set the parameter field, and output files are different (see Figure 1). The meaning of each scan mode is as follows.

ConstZ: constant-height mode. The force acting on the tip that is scanned at a constant height is calculated.

ConstForce: constant-force mode. The tip height is searched so as to the force acting to the probe is equal to the value of the specified one. To find the proper height, the tip is scanned the range from the initial position of the tip to the length specified by “scanarea-h”. If there is no proper height during this, the lowest point of the range is outputted. On the calculation in the aquatic environment, you cannot calculate in this mode.

ncAFM-ConstZ: Non-contact mode height constant. To scan the plane at a constant height while vibrating the probe to calculate the forces acting

on the probe. In addition to the force acting on the probe, the output frequency shift or the amount of energy dissipation.

ForceCurve: Force curve measurement mode. Close to the sample probe in the xy position there, to calculate the forces acting on the probe.

MinForceHeight: minimum power mode. In each position on the plane to locate the height of the probe to minimize the forces acting on the probe. To explore the range in height from the initial position of the tip "scanarea - h" is set in the range. On the calculation in the aquatic environment, you cannot calculate in this mode.

				scanmode				
				ConstZ	Const Force	ncAFM-ConstZ	Force Curve	MinForce Height
input			scanarea – w scanarea – d	○	○	○	-	○
			scanarea – h	-	○	○	○	○
	Tip_Control		delta_xy	○	○	○	-	○
			delta_z	-	-	-	○	-
		NC_Mode_Setting	ThetaStepNumber	-	-	○	-	-
			TipZamplitude	-	-	○	-	-
			SpringConst	-	-	○	-	-
			ResoFreq	-	-	○	-	-
			ForceConst	-	○	-	-	-
			OneWayForceCurve	-	-	-	○	-
			nonElectroStatic	○	○	○	○	○
output	Output		Fx	○	○	※1	○	○
			Fy	○	○	※1	○	○
			Fz	○	○	※1	○	○
			FrequencyShift_2D	-	-	○	-	-
			EnergyDissipation_2D	-	-	○	-	-
			TipPositionZ	-	○	-	-	○
			Movie	○	○	○	○	○
			Log	○	○	○	○	○

Figure.1 Input and output of each scan mode.

※1 The result file is not displayed properly on the software.

delta_xy

Pixel size of xy-direction. Angstrom unit.

delta_z

Pixel size of z-direction. Angstrom unit.

NC_Mode_Setting - ThetaStepNumber

"n" value in figure 2. The larger you set this value, the more improved the accuracy is.

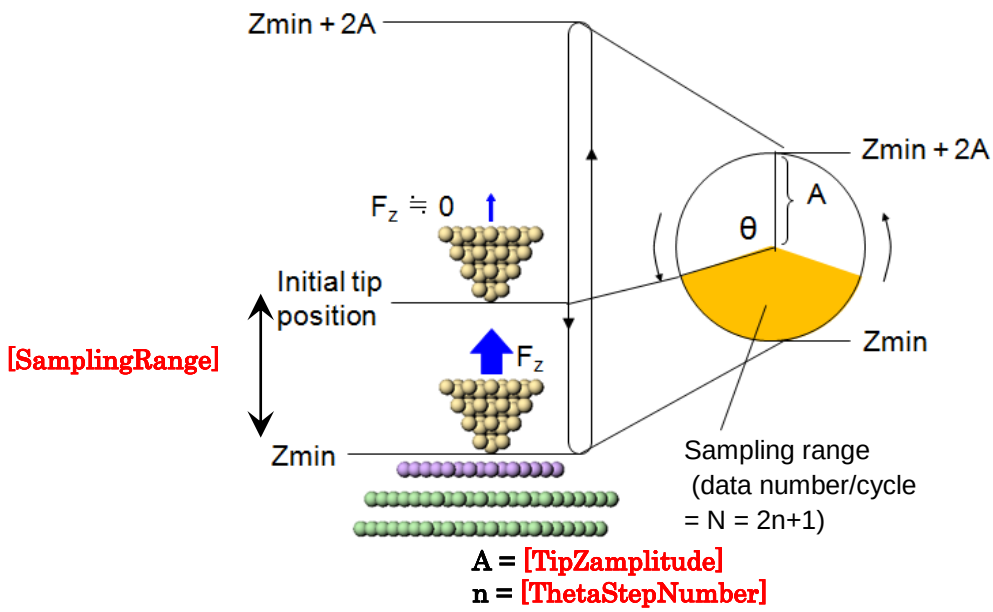


Figure.2 Image of the calculation method of nc-AFM mode.

NC_Mode_Setting - TipZamplitude

Amplitude of the tip of the cantilever. Angstrom unit.

NC_Mode_Setting - SpringConst

Spring constant of the cantilever.

NC_Mode_Setting - ResoFreq

Resonance frequency of the cantilever.

NC_Mode_Setting - FreqShift

Frequency shift. Hz unit.

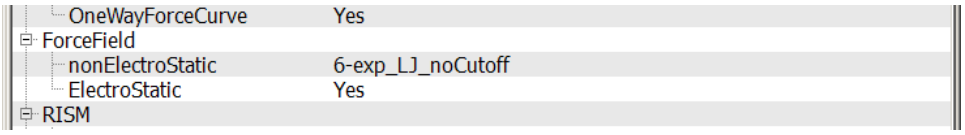
ForceConst

Force.

resetStructure_atZmax

Each x of the tip at the position y, after the end of the calculation, set whether to restore the structure of the sample molecules. If set to yes back to the original structure, no, if you set the probe to move the structure intact.

OneWayForceCurve



ForceField：Parameters for the interaction between a tip and samples.

nonElectroStatic

Functional form for the van der Waals interaction between a tip and samples. You can use either 6-exp type function, which is adopted to the MM3 force field, or 6-12 type of the Lennard-Jones function. Moreover, you can choose whether to consider the interaction between atoms on far distance each other or not.

6-exp_LJ_noCutoff

In order to calculate the van der Waals interaction, the simulator uses the 6-exp type MM3 function. The simulator calculates the interactions for all the pairs between the atoms.

6-exp_LJ_withCutoff

In order to calculate the van der Waals interaction, the simulator uses the 6-exp type MM3 function. The simulator calculates the interactions for the pairs whose distance is larger than 2.3 times the specific distance.

6-12_LJ_noCutoff

In order to calculate the van der Waals interaction, the simulator uses the 6-12 type Lennard-Jones function. The simulator calculates the interactions for all the pairs between the atoms.

6-12_LJ_withCutoff

In order to calculate the van der Waals interaction, the simulator uses the 6-12 type Lennard-Jones function. The simulator calculates the interactions for the pairs whose distance is larger than 2.3 times the

specific distance.

ElectroStatic

Whether considering the Coulomb interaction between a tip and samples or not.

ElectroStatic	Yes		
RISM			
TypeOfFourierTransform	log		linear/log
Temperature	298.0	K	
NumberOfRadiusBin	512		
LogRadiusMin	-4.37	ln(rmin/Ang)	log Fourier Trans. only
DeltaLogRadius	0.021	delta ln(r/Ang)	log Fourier Trans. only
VolumeRadius	10	Ang	linear Fourier Trans. only
Solvent			
Molecule	water		water only
NumberDensity	0.03334	Ang^(-3)	
Solvent_Solvent			
InitialBroadening	1.4	Ang	
Tolerance	0.0001		
RISMStepMax	1000		
Solute_Solvent			
InitialBroadening	1.5	Ang	
Tolerance	0.0001		
RISMStepMax	1000		
Output			

RISM：Parameters for the calculation in the aquatic environment

TypeOfFourierTransform

Scale of the variable for the numerical Fourier transform. You can choose either the linear scale or the logarithmic one.

Temperature

Temperature of the water. K unit.

NumberOfRadiusBin

Number of the data points for the numerical Fourier transform. Recommended to set the value to the power of 2.

LogRadiusMin

Minimum of the variable for the numerical Fourier transform in logarithmic scale. The value is equal to ln([minimum in the linear scale]/Angstrom).

DeltaLogRadius

Minimum distance between the data points for the numerical Fourier transform in logarithmic scale.

VolumeRadius

Maximum of the variable for the numerical Fourier transform in linear scale. Angstrom unit.

Solvent - Molecule

Type of the solvent. Only water in this version, and you cannot change it.

Solvent - NumberDensity

Number density of the solvent, that is to say, water. (Angstrom)^(-3) unit.

Solvent _Solvent - InitialBroadening

Parameter, σ, of the initial form of the direct correlation function when the solver calculates the solvent-solvent distribution function. (Angstrom)^(-1) unit. The initial form is $c_{\alpha\gamma}^{(0)}(r) = -\beta\, q_\alpha q_\gamma \left[1 - \exp(-\sigma r)\right]/r$, for the interaction site between α and γ. The symbol $\beta = 1/k_{\mathrm{B}} T$ is the inverse temperature. The symbols q_α and q_γ are the charges of the interaction sites. (You do not need to set the value of these symbols here.) The symbol r is the distance between the sites.

Solvent _Solvent - Tolerance

Tolerance for the calculation of the solvent-solvent distribution function. The solver stops calculating when the average value of the distribution function on the data points is achieved to the value of this tolerance. Non-dimensional value.

Solvent _Solvent - RISMStepMax

Maximum of the iteration number for the calculation of the solvent-solvent distribution function. The solver stops calculating the distribution functions when the iteration number exceeds this maximum, even If the tolerance is not achieved.

Solvent _Solute - InitialBroadening

Parameter of the initial form of the direct correlation function when the solver calculates the soulte-solvent distribution function. (Angstrom)^(-1) unit. The initial form is the same as the solvent-solvent functions.

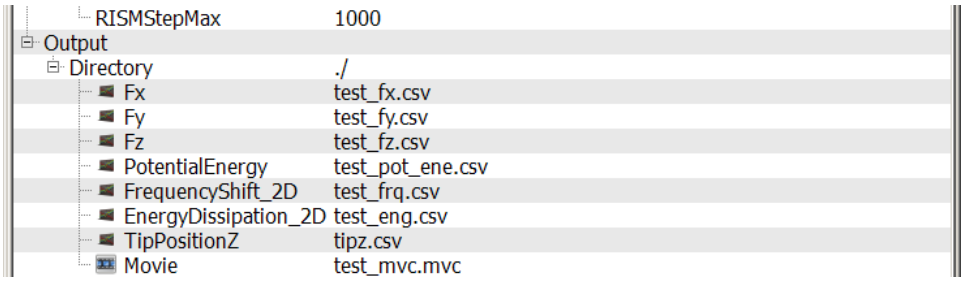
Solvent _Solute - Tolerance

Tolerance for the calculation of the solute-solvent distribution function. The solver stops calculating when the average value of the distribution function on the data points is achieved to the value of this tolerance. Non-dimensional value.

Solvent _Solute - RISMStepMax

Maximum of the iteration number for the calculation of the solute-solvent distribution function. The solver stops calculating the distribution functions

when the iteration number exceeds this maximum, even If the tolerance is not achieved.



RISMStepMax	1000
Output	
Directory	./
Fx	test_fx.csv
Fy	test_fy.csv
Fz	test_fz.csv
PotentialEnergy	test_pot_ene.csv
FrequencyShift_2D	test_frq.csv
EnergyDissipation_2D	test_eng.csv
TipPositionZ	tipz.csv
Movie	test_mvc.mvc

Output：Parameters of output files. All of them cannot be edit.

Fx

x-component of force to tip. Newton unit.

Fy

y-component of force to tip. Newton unit.

Fz

z-component of force to tip. Newton unit.

PotentialEnergy

Total energy of the system (In the calculation for the environment in water, total free energy of the system.) eV unit.

FrequencyShift_2D

frequency shift image.

EnergyDissipation_2D

energy dissipation image.

TipPositionZ

tip height image. Angstrom unit.

Movie

animation file

【trouble shooting】

◆ did not find vdw parameter.

The input of the simulation model includes the improper element that is not covered by MM3 force field. For more information, see the chapter 4.2 of the tutorial for more

information.

◆ did not find force field parameter.

The input of the simulation model includes the improper structure that is not covered by MM3 force field.

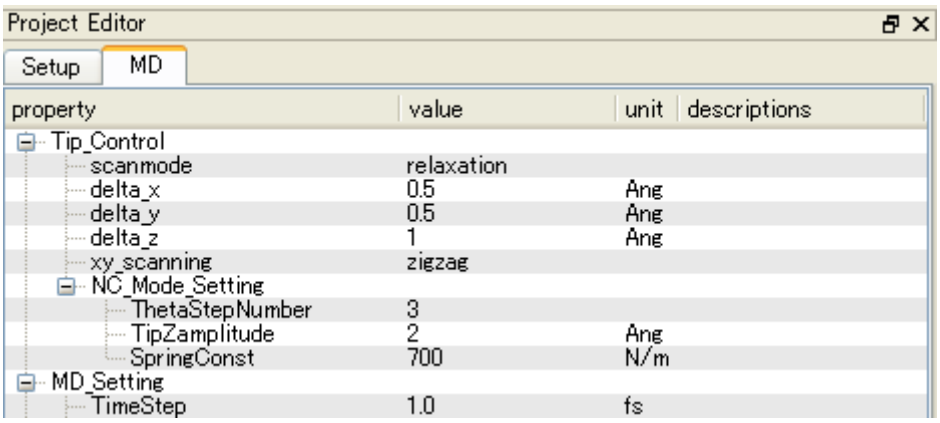
Input of the MD-AFM simulator

This simulator will make you simulate AFM image by calculating the tip-sample interaction and the sample deformation. Calculation procedure is roughly as follows.

① Setting the tip position.
② Calculate the force acting to the tip.
③ Move the tip to the next position.
2-3 are repeated.

By setting the input parameters explained below, you can control the procedure of these calculation.

For specifying the parameter of “MD-AFM Simulator”, you first select the “MD” tag of the Project Editor. This tag has four columns there.



• “property” is the name of the parameter.

• “value” is the value of the parameter.
• “unit” is the unit of the parameter.
• “descriptions” is the notes of the setting parameters.

In the following, detailed description of the meaning of each item of “property” column.

Tip_Control		
scanmode	relaxation	
delta_x	0.5	Ang
delta_y	0.5	Ang
delta_z	1	Ang
xy_scanning	zigzag	
NC_Mode_Setting		
ThetaStepNumber	3	
TipZamplitude	2	Ang
SpringConst	700	N/m

Tip_Control：the parameters for control the probe tip.

scanmode

Scan mode of the probe tip selected from “ConstZ”, “ConstForce”, “ncAFM-ConstZ”, “ForceCurve” or “MinForceHeight”. The selected scan mode, you can set the parameter field, and output files are different (see Figure 1). The meaning of each scan mode is as follows.

ForceCurve：Force curve measurement mode. Close to the sample probe in the xy position there, to calculate the forces acting on the probe.

ConstZ：constant-height mode. The force acting on the tip that is scanned at a constant height is calculated.

NC-ConstZ：Non-contact mode height constant. To scan the plane at a constant height while vibrating the probe to calculate the forces acting on the probe. In addition to the force acting on the probe, the output frequency shift or the amount of energy dissipation.

relaxation：Calculation of structural relaxation.

				scanmode			
				ForceCurve	ConstZ	NC_ConstZ	relaxation
Input		delta_x		-	○	○	-
		delta_y		-	○	○	-
		delta_z		○	-	-	-
		xy_scanning		-	○	○	-
	Tip_Control	NC_Mode_Setting	ThetaStepNumber	-	-	○	-
			TipZamplitude	-	-	○	-
			SpringConst	-	-	○	-
	MD_Setting	TimeStep		○	○	○	○
		StepNumber		○	○	○	○
		Temperature		○	○	○	○
		Safety_mode		○	○	○	○
		Initial_Velocity		-	-	-	-
output	Output	Fx		○	○	※1	-
		Fy		○	○	※1	-
		Fz		○	○	※1	-
		FrequencyShift_2D		-	-	○	-
		EnergyDissipation_2D		-	-	○	-
		Energy		○	○	○	○
		energy_freq		○	○	○	○
		Movie		○	○	○	○
		movie_freq		○	○	○	○

Figure.1 Input and output of each scan mode.

※1 The result file is not displayed properly on the software.

delta_x

Pixel size of x-direction. Angstrom unit.

delta_y

Pixel size of y-direction. Angstrom unit.

delta_z

Pixel size of z-direction. Angstrom unit.

xy_scanning

method of scanning of xy-direction.

NC_Mode_Setting - ThetaStepNumber

"n" value in figure 2. The larger you set this value, the more improved the accuracy is.

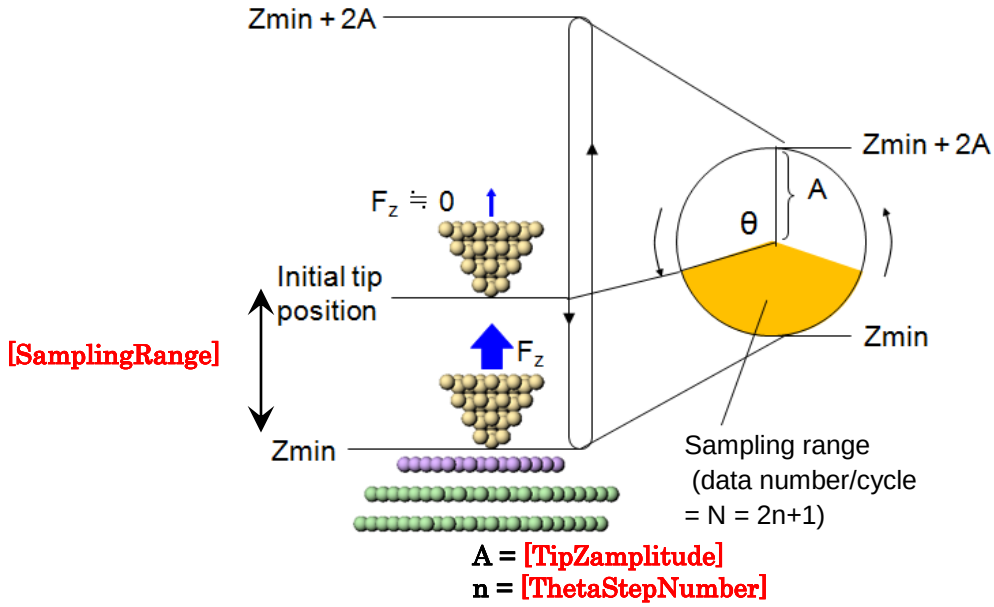


Figure.2 nc-AFM mode

NC_Mode_Setting - TipZamplitude

Amplitude of the tip of the cantilever. Angstrom unit.

NC_Mode_Setting - SpringConst

Spring constant of the cantilever.

MD_Setting		
TimeStep	1.0	fs
StepNumber	10000	
Temperature	300	K

MD_Setting：The parameter of molecular dynamics calculation.

TimeStep

Value of time step. fs unit.

StepNumber

The number of MD step per one tip position.

Temperature

temperature. K unit.

ForceField：The parameter about the calculation of the

Safety_mode

If the file of MM3 force field parameter don't include the parameter of the tip or the sample input model,

stopCalc：don't calculate.

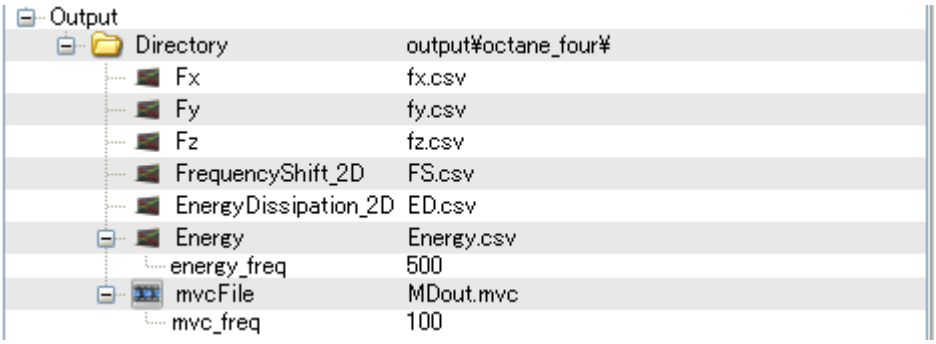
setZeroParam：If the MM3 force field parameter is not exist, the value of the parameter is set to zero.

fixMolecule：The simulator make you calculate not considering the deformation of the molecule.

Input：input file

Initial_Velocity

Input file of the initial velocity of each atoms.



Output：

Directory

output directory

Fx

x-component of force to tip. Newton unit.

Fy

y-component of force to tip. Newton unit.

Fz

z-component of force to tip. Newton unit.

FrequencyShift_2D

frequency shift image.

Energy

energy of the system. kcal/mol unit

Movie

animation file

【trouble shooting】

- cannot open FF parameter file.

  You have to place the parameter file to proper directory. See the the chapter 1.2 of the tutorial for more information.

- "TipZamplitude" must be smaller than "scanarea.z/2."

  You have to decrease the value of TipZamplitude” or increase that of ” scanarea.z”.

- Atom mass is not defined properly.
- did not find vdw parameter.

  The input of the simulation model includes the improper element that is not covered by MM3 force field. For more information, see the chapter 4.2 of the tutorial for more information.

- did not find Force Field Parameter.

  If ”Safety_mode” is set to ” stopCalc” and the input of the simulation model includes the improper element that is not covered by MM3 force field, you cannot simulate. In this case, you have to set ” Safety_mode” to ” setZeroParam” or ” fixMolecule”.

- warning: atom[ID] is unstable.

  Calculation of molecular dynamics is unstable. You have to decrease the value of “TimeStep” or set parameter not to narrow the distance between the tip and the sample too closely.

5. Quantum Mechanical SPM Simulator

Note on the input parameter in Setup tab

Please pay attention that there are the following limits on the input parameters in Setup tab, when we use our Quantum Mechanical SPM Simulator.

- We need that there are one 'Tip' tag and one 'Sample' tag in the 'Component' tag. When there is an 'Image' tag, we cannot start to calculate.

- We can only use the following kind of files on the 'Tip' tag:
  - whose extension is either txyz or xyz
  - the set of the atoms exists in 'two_body_parameter_folder'.

- Also, we can only use the following kind of files on the 'Sample tag:
  - whose extension is either txyz or xyz
  - the set of the atoms exists in 'two_body_parameter_folder'.

- The amount of the available memory in your PC decides the limit of the total number of atoms in the system (and the limit of k-points for samples' Brillouin zone in DFTB_STM/DFTB_STS).

- The values which affect the calculation are those in the following tags: Position, Rotation, ScanArea, DistanceFromSamples. The values in the 'Property' tag do not affect the calculation by this Simulator.

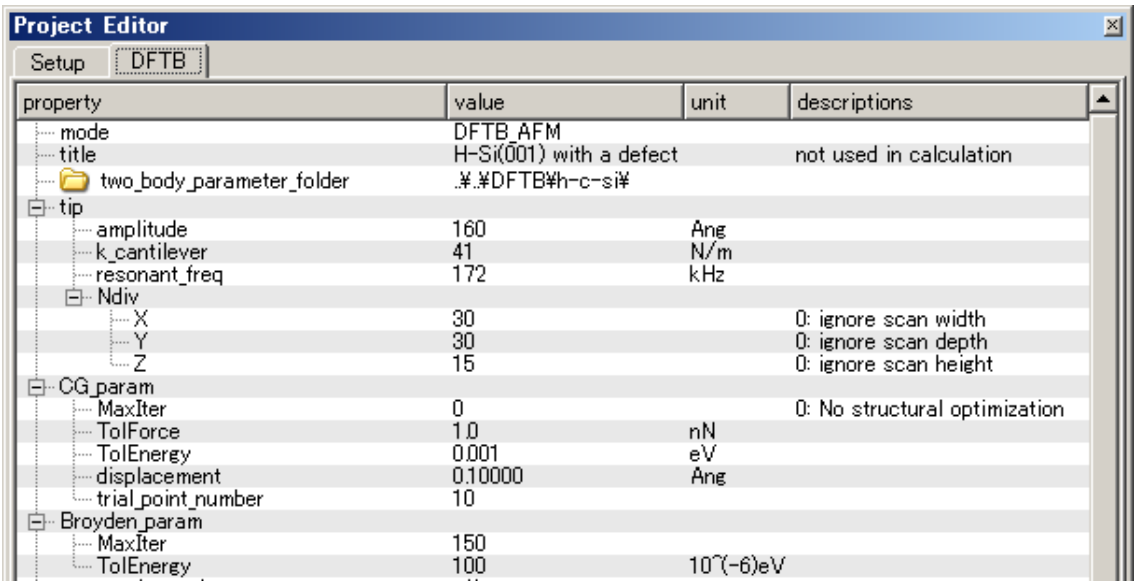
- (In case of AFM calculation,) we need to set the value of 'ScanArea - h' tag smaller than the twice of the value of 'tip - amplitude' tag in 'DFTB' tab, which we will describe the next section.

- (In case of STM constant current calculation,) we need to set the value of 'ScanArea - h' tag to set the tip's lowest position from initial height in a feedback loop. When the tip cannot find out the height to coincide with the set point current "set_point", tip's height is determined to be (initial height of the tip) – ('ScanArea - h') on the

topographic image.

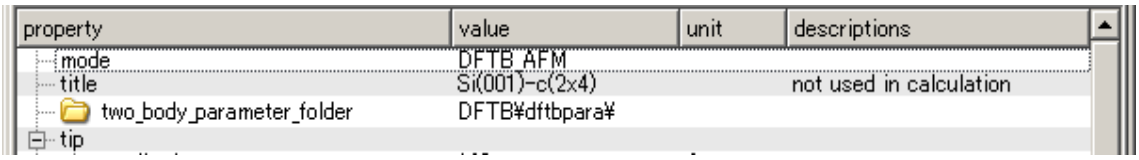
Input parameters in DFTB tab

We can set the input parameters for our “Quantum Mechanical SPM Simulator” from the ‘DFTB’ tag panel in the ‘Project Editor’. There are four columns in this tag.



- The ‘property’ column denotes the name of the parameter.
- The ‘value’ column denotes the input value of the parameter.
- The ‘unit’ column denotes the unit of the parameter (if it exists).
- The ‘descriptions’ column denotes the brief comment for the parameter.

We describe the precise meaning of the input parameters below.



Parameters related to the whole calculation

mode

Calculation mode in “Quantum Mechanical SPM Simulator”. We can choose it from among the following list: DFTB_AFM, DFTB_STM, DFTB_STS, DFTB_KPFM, and DFTB_BAND. These correspond to the simulation of atomic force microscopy, that of tunnelling current microscopy, that of tunnelling current spectroscopy, that of Kelvin probe microscopy, and band calculation of a sample respectively.

title

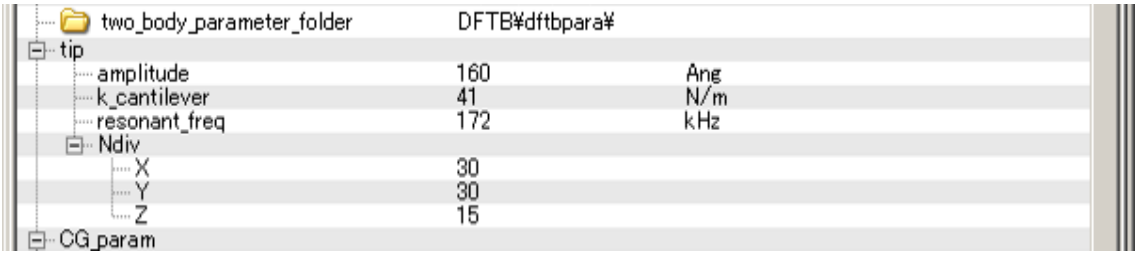
Title of this simulation project. We can write the arbitrary sentence. This value does not affect the calculation result.

two_body_parameter_folder

The folder name which contains the data for interaction between two atoms. The folder name is fixed.

stm_mode

Calculation mode in STM calculation. We can choose it from among the following list ConstantHeight and ConstantCurrent. ‘ConstantHeight’ corresponds to the conctant height mode and ‘ConstantCurrent’ corresponds to the constant current mode. This content makes a sense only when we choose DFTB_STM mode.



tip：Parameters for tip and cantilever

amplitude

Amplitude of the tip (the top of the cantilever). We use it when we want to calculate the value of the frequency shift in the ‘DFTB_AFM’ mode. We need to set its value larger than the half of the value of the ‘Tip - ScanArea - h’ tag in ‘Setup’ tab.

k_cantilever

Spring constant of the cantilever. We use it when we want to calculate the

value of the frequency shift in the ‘DFTB_AFM’ mode.

resonant_freq

Resonant frequency of the tip (the top of the cantilever). We use it when we want to calculate the value of the frequency shift in the ‘DFTB_AFM’ mode.

Ndiv - X

Division number of the x-axis direction in the scanning region. When we set it to 0, we reset the width of the scanning region to 0. In case of the ‘DFTB_STS’ mode, we force to set the value of this parameter to 0.

Ndiv - Y

Division number of the y-axis direction in the scanning region. When we set it to 0, we reset the depth of the scanning region to 0. In case of the ‘DFTB_STS’ mode, we force to set the value of this parameter to 0.

Ndiv - Z

Division number of the y-axis direction in the scanning region. When we set it to 0, we reset the height of the scanning region to 0. In case of the ‘DFTB_STS’ mode, we force to set the value of this parameter to 0.

Z	15		
CG_param			
MaxIter	0		0: No structural optimization
TolForce	1.0	nN	
TolEnergy	0.001	eV	
displacement	0.10000	Ang	
trial_point_number	10		
Broyden_param			

CG_param：Parameters for structure relaxation

MaxIter

Maximum of the iteration number for structure relaxation. When we set it to 0, the calculation of structure relaxation is not done.

TolForce

Threshold for the force per atom in order that we decide whether the structure is fully relaxed.

TolEnergy

Threshold for the difference of the total energy in order that we decide whether the structure is fully relaxed.

displacement

Maximum of the displacement of atoms when we search the relaxed position.

trial_point_number

Number of the history of the result data used for the next search of the relaxed structure.

trial_point_number	10		
Broyden_param			
MaxIter	150		0: No structural optimization
TolEnergy	100	10^(-6)eV	
output_eigenvalue	off		on/off
Fvdw			

Broyden_param：Parameters of the electronic states calculataion

MaxIter

Maximum of the iteration number for electronic states calculation. When we set it to 0, the calculation of the electronic states is not done.

TolEnergy

Threshold for the difference of the total energy in order that we decide whether the electronic state is fully converged.

output_eigenvalue

Whether output the values of the eigenenergy of the system. (The values are only for the Γ point in the Brillouin zone.) ‘on’ is output, and ‘off’ is not ouput.

output_eigenvalue	off		on/off
Fvdw			
tip_shape	conical		
height_of_highest_adsorbed_molecule	0.00000	Ang	
Hamaker_const	0.22	aJ/mol	
apex_angle	120	degree	
tip_height	1000	Ang	
radius_of_tip_apex	1.00000	Ang	
tip_bias_voltage			

Fvdw：Parameters of the macroscopic shape of the tip

tip_shape

Macroscopic shape of the tip. We can choose one from the following list: pyramidal/parabolic/spherical/conical.

height_of_highest_adsorbed_molecule

Maximum height of the adsorbed molecule.

Hamaker_const

Hamaker constant of the tip. ‘aJ’ in the unit column means 10^(-18) J.

apex_angle

Tip apex angle. It is available in case of pyramidal and conical shape.

tip_height

Height of the tip. It corresponds the diameter in case of spherical shape.

radius_of_tip_apex

Curvature radius of the tip apex. It is available in case of conical shape only. In case of spherical shape, we use the value of tip_height/2, not the value specified here.

radius_of_tip_apex	1.00000	Ang
tip_bias_voltage		
minimum	-1.00000	V
maximum	1	V
Ndiv	0	
electron_temperature	50	K
tip_charge_neutrality		

feedback_param:

Parameters for feedback loop. These parameters make a sense only when there are feedback loops.

delta_z

Maximum z-direction movement of a tip in the feedback loop.

set_point

A current set point for the feedback loop. The value is absolute value and should be positive. Because of the calculation method, you may set a very different value from an experimental set point value to gain valid topographical image, for example, you should set 2000nA to this value when experimental value is 0.3nA. You may guess the range of valid value by taking the range of the current of a valid constant height mode image which will be gained by varying the tip-sample distance.

TolCurr

Threshold for the difference between a ‘set_point’ and calculated current in order that we decide whether the tip has reached a valid z-position in a feedback loop. This value should be smaller than the value ‘set_point’.

MaxIter

Maximum of the iteration number for the feedback loop.

tip_bias_voltage : Parameters of tip bias. Available only for DFTB_STM/DFTB_STS mode.

(Assume that the sample bias is 0.)

minimum

Minimum value.

maximum

Maximum value.

Ndiv

Division number between ‘minimum’ and ‘maximum’ (in DFTB_STS mode). When we set it to 0, the value of ‘minimum’ is used. In DFTB_STM mode, this parameter forces to be set to 0.

Ndiv_kpoints

(In DFTB_STM/DFTB_STS mode only.)Division number of k-points in samples’ Brillouin zone. In calculation of samples’ states, we take ‘Ndiv_kpoints’ times ‘Ndiv_kpoints’ k-points in 2-dimensional Brillouin zone. This value should be positive even integer.

DoS

Parameters for calculation of density of states of sample surface (in DFTB_STM mode only).

output_dos

Whether we calculate the DoS of the sample surface or not.

minimum

Minimum value of energy range for DoS calculation.

maximum

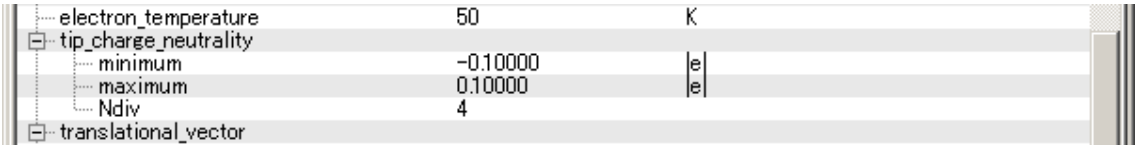
Maximum value of energy range for DoS calculation.

Ndiv

Division number between ‘minimum’ and ‘maximum’.

electron_temperature

Electron temperature of the system.



electron_temperature	50	K
tip_charge_neutrality		
minimum	-0.10000	|e|
maximum	0.10000	|e|
Ndiv	4	
translational_vector		

tip_charge_neutrality：Parameters of tip charge neutrality. Available only for DFTB_KPFM mode. The value of sample charge neutrality has the same absolute value as the tip one, and an opposite sign of the tip one. (We assume that the whole system is electrically neutral.) The reason why the charge neutrality is the input parameter describes the document of the calculation model.

minimum

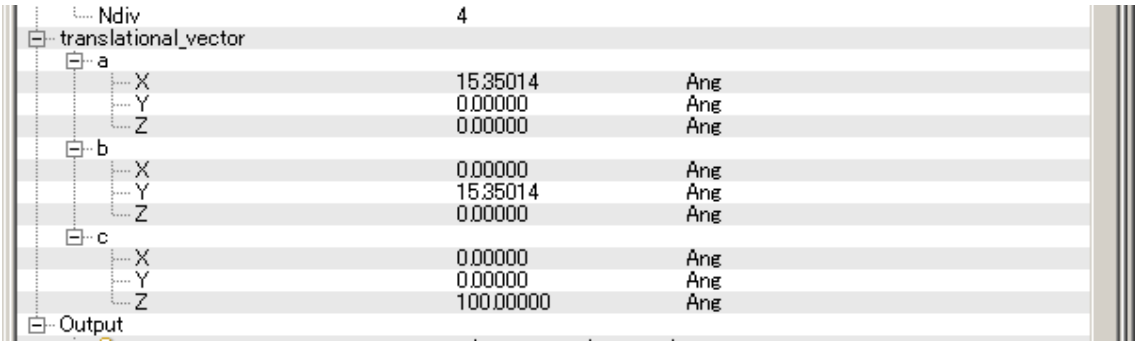
Minimum value. Its unit is the elementary charge.

maximum

Maximum value. Its unit is the elementary charge.

Ndiv

Division number between ‘minimum’ and ‘maximum’ . When we set it to 0, the value of ‘minimum’ is used. In case that we want to calculate the image of the local contact potential difference, please set it to be larger than 3.



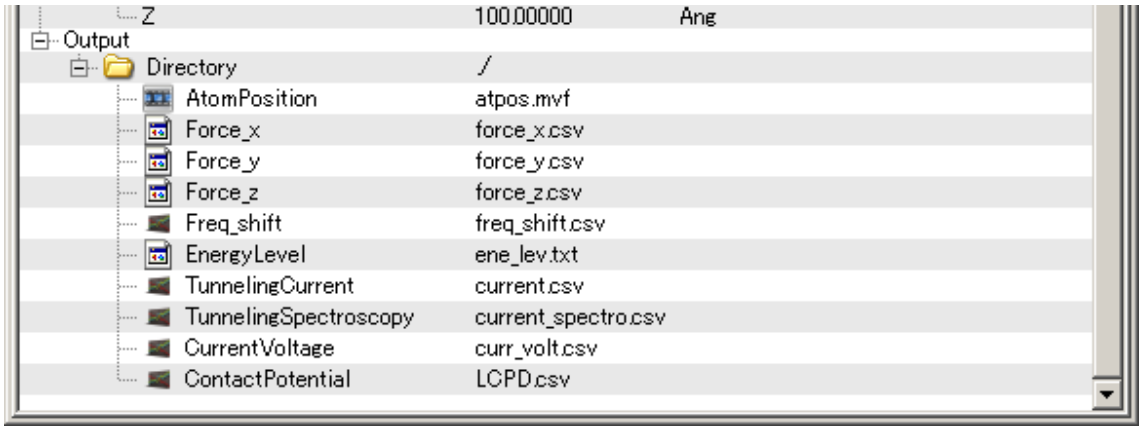
Ndiv	4	
translational_vector		
a		
X	15.35014	Ang
Y	0.00000	Ang
Z	0.00000	Ang
b		
X	0.00000	Ang
Y	15.35014	Ang
Z	0.00000	Ang
c		
X	0.00000	Ang
Y	0.00000	Ang
Z	100.00000	Ang
Output		

OpenMP_threads

The number of CPUs for the parallel computing.

translational_vector：Unit lattice vector

The vector c is only used for three-dimensional calculation in DFTB_BAND mode.



band_calculation

Parameters for band calculation (in DFTB_BAND mode only).

lattice_type

Names of lattice types. The names with the head '2D_' correspond to two dimensional lattice.

band_kpoints

The division number of k-points in sample's Brillouin zone. If we think N as this number, the number of k-point is N times N in two dimensional band calculation and N times N times N in three dimensional band calculation. If a band calculation you try to do takes too much memory, you should reduce this value.

CAUTION: You should set even number for this parameter.

band_ndiv

The division number of plotted lines in a calculated band structure.

Output：Parameters of output files. All of them cannot be edit.

Directory

Output directory name. This indicated that the files are outputted to the directory in which the project files are saved.

All the following parameters describe the output file name. These are also used as the labels in ‘Result view’. Only the files that is suitable for the calculation mode are generated. The meaning of the data in each file is as follows:

AtomPosition

Data for animation of the atom configuration. (Since this file is binary format one, we cannot see the value of the data directly.)

Force_x, Force_y, Force_z

Value of the x, y, and z component of the force exerted on the tip in each tip position. Although these files are not suitable for visualization by our GUI, we can see the value of the data. (We record the coordinate of the tip, the phase of the tip, the component of the force, the tip charge neutrality (in case of the KPFM mode).)

Freq_shift

Value of the frequency shift at each tip scanning position. Its unit is Hz. We can see the two-dimensional map of this data by the ‘Result view’.

EnergyLevel

Value of the eigenenergy. Although this file is not suitable for visualization by our GUI, we can see the value of the data.

TunnelingCurrent

Value of the tunneling current at each tip position. Its unit is nA. We can see the two-dimensional map of this data by the ‘Result view’.

STM_topography

The height of the tip in STM constant current mode. Its unit is angstrom. We can see the two-dimensional map of this data on the ‘Result view’.

TunnelingSpectroscopy

Value of the tunneling current spectroscopy ((dI/dV)/(I/V)) corresponding to the tip bias. The unit of the bias is V. We can see the line graph of this data by the ‘Result view’.

CurrentVoltage

Value of the tunneling current corresponding to the tip bias (so-called I-V curve). The unit of the current and the bias is nA and V, respectively. We can see the line graph of this data by the ‘Result view’.

DoS

Density of states of the sample surface corresponding to the energy. The unit of the energy is eV and the unit of the density of states is 1/eV. We can see the line graph of this data on the ‘Result view’.

ContactPotential

Value of the local contact potential difference at each tip position. Its unit is eV. We can see the two-dimensional map of this data by the ‘Result view’.

BandStructure

A Band structure of a sample. The unit of vertical component if eV.

Typical error message and their solution

The messages are aligned in the alphabetical order.

- *Array allocation error; ...* : It means that the total amount of the memory which needs to be used in calculation exceeds that of the available memory in your PC. Please decrease the value of input parameters (maybe, the number of the atoms in tip and/or sample structure files).

- *Error: cannot open the following file. C:¥(folder name)¥atoms* : It means that the simulator cannot find the input files corresponding to the setting of 'two_body_parameter_folder' tag. Please check that the directory named C:¥(folder name) exists.

- *Error: tip data file not found. Stopped.* : It means that the setting of tip in Setup tab is wrong.

- *Niter reaches MaxIter in BR process.* : It is displayed when the target value cannot be reached on the iterative calculation of the electronic state. Please be larger the target value and/or the maximum number of the iteration.

- *qionmax is out of range for input [cini:cfin]. (decimal value), or Some qionmax are out of range for input [cini:cfin].* : It is possible that the estimation of the contact potential difference is not suitable. (Precisely, this message means that the extremum position estimated by the fit to the quadratic function is out of the range of [cini:cfin]. (The values of the cini and cfin are ones of tags of

tip_charge_neutrality - minimum and tip_charge_neutrality - maximum.) Please change their values and calculate again. As for the algorithm of the estimation of the contact potential difference, see the document of the calculation model.

- *The eigenvalue equation cannot be solved. Stopped. It may be because some atoms are set too close.* : It means that the simulator cannot calculate the eigenvalue equations in the electronic state calculation. This may occur when there are the pairs of atoms with a small distance. Please check the data in the structure files of the tip and sample, and the value of the distance between them. When you have render the simulation with structure relaxation, you may avoid this error by setting the value of the tag 'CG_param - displacement' to be smaller one.

When you see the messages which are not listed here, please contact our support with the message.