A table of functions of the SPM simulator

How to use solvers included in the package effectively

Advanced Algorithm & Systems

Analyzer	The Experimental Image Data Processor
GeoAFM	The Geometrical Mutual AFM simulator
FemAFM	The Finite Element Method AFM Simulator
LiqAFM	The Soft Material Liquid AFM Simulator
macroKPFM	The Macroscopic KPFM Simulator
CG	The Geometry Optimizing AFM Image Simulator
MD	The Molecular Dynamics AFM Image Simulator
DFTB	The Quantum Mechanical SPM Simulator
SetModel	The Sample Modeling

In this document, we show some typical examples for each solver.
Reading this document, you can select a suitable solver for simulating your own problem.

An outlook of the SPM simulator

Case examples for each solver

Solver	Characteristics	Functions
Analyzer: The Experimental Image Data Processor	A preprocessor for simulations. This solver transforms the experimental data into input data for calculations. It removes artifacts made by imperfect tips from experimental images.	(1) The blind tip reconstruction method (2) Importing the experimental binary data files in various formats (3) Modifying a tilt of the experimental image
SetModel: The Sample Modeling	A preprocessor for simulations. This solver prepares input data of models made from atoms for the tips and the samples.	(1) Preparing periodic structures of atoms for thin layers of semiconductors (2) Putting impurity atoms into thin layers of crystals (3) Construction of hydrogen-terminated surfaces
GeoAFM: The Geometrical Mutual AFM simulator	A solver for the AFM simulations in the mesoscopic and macroscopic scales. It works as a three-way data processor, so that it reconstructs the one out of the other two among three geometrical elements, a tip, a sample material and its AFM image. Simulation results are not exact, but they are obtained rapidly.	(1) Constructing an AFM image from data of shapes of a tip and a sample (2) Constructing an image of a sample from an experimental AFM image and data of a shape of a tip (3) Constructing an image of a tip from an experimental AFM image and data of a shape of a sample (4) It is suitable for analyzing collagens and proteins.

Suitable for engineers in practical uses

Suitable for engineers in practical uses

FemAFM: The Finite Element Method AFM Simulator	This solver simulates the AFM image with approximating the sample and the tip as models of continuous elastic medium. Simulation results are effective in mesoscopic and macroscopic scales. Functions of the DLVO theory are included.	(1) Simulating both the vertical motion and the twist motion of the cantilever (2) Obtaining the resonant frequency of the motion of the cantilever for the vacuum environment, the air environment, and the liquid environment. (3) Functions of the DLVO theory are included
LiqAFM (tapping): The Soft Material Liquid AFM Simulator	This solver simulates the motion of the cantilever, the viscoelastic contact dynamics on the surface of the sample, and tapping of the tip over the surface of the sample material in the liquid environment. It is suitable for examining soft and bio-related materials, for example, proteins.	(1) Simulating both the vertical motion and the twist motion of the cantilever (2) Obtaining the resonant frequency of the motion of the cantilever for the vacuum environment, the air environment, and the liquid environment. (3) Suitable for analyzing collagens and proteins (4) The LiqAFM can solve the inverse problem, so that it derives Young's modulus and the surface tension from the frequency shift and the phase shift. (Reference)
macroKPFM: The Macroscopic KPFM Simulator	This solver examines the KPFM images in micrometer and nanometer scales. It carries out the simulations by solving the problem of electric potential classically according to the boundary element method.	(1) This solver can treat the dielectric materials in arbitrary shapes. (2) This solver can simulate arbitrary distribution of the point charges on the surface of dielectric materials. (3) It is suitable for examining the polymers.

Suitable for researchers

CG: The Geometry Optimizing AFM Image Simulator	This solver finds optimized configuration of atoms in the tip and the sample by classical method. To solve the problem in the liquid environment, you can use the CG-RISM solver.	(1) This solver can examine the dissipation of the energy, the frequency shift images, and the force curves. (2) The constant height mode is available. (3) The constant force mode with contact between the tip and the sample is available. (4) It is suitable for analyzing collagens and proteins.
MD: The Molecular Dynamics AFM Image Simulator	This solver examines the molecular dynamics of the tip and the samples with classical method.	(1) This solver can obtain force curves. (2) It calculates force fields, energy dissipation, and the frequency shift images. (3) This solver can predict the sample material's deformation caused by the interaction between the tip and the sample material. (4) It is suitable for analyzing collagens and proteins.
DFTB: The Quantum Mechanical SPM Simulator	This solver examines the tunnel currents between the tip and the sample with the quantum mechanics. It simulates STM/STS, AFM, and KPFM.	(1) This solver simulates the AFM images, the STM images, and the KPFM images. (2) To obtain the STM images, both constant height mode and the constant current mode are available. (3) This solver can calculate the band structure of sample materials, for example, metals and semiconductors. (4) It solves problems according to the DFTB (Density Functional based Tight Binding) Method. (5) This solver aims at collaboration with the PHASE/0. (Reference)

バイオ・ソフトマテリアル関連ユーザー向けに、新たに追加された機能

LiqAFMタッピング機能

探針-試料間の粘弾性凝着効果を考慮したスキャン

LiqAFMタッピング・モードの逆問題計算機能

周波数シフト・位相シフトの観測データより、試料のヤング 率、表面張力、高さ情報を逆算

FemAFM_DLVO機能

探針・試料が電解溶液中にあるとして、電気二重層力の効果に よるデバイ遮蔽効果を評価
ファンデルワールス力と、電気二重層による斥力の、二つの力 の競合を調べる

macroKPFM_DLVO機能

探針・試料が電解溶液中にあるとして、電気二重層力の効果 によるデバイ遮蔽効果を評価
ファンデルワールス力と、電気二重層による斥力の、二つの 力の競合を調べる

今後の展開としては、逆問題機能が残されている

株式会社XXXXXX様への対応

XXXXXXでは、誘電率、分極など、様々な試料・探針の電気特性に興味を 持っている。例えば、金属基板に試料を乗せ、探針でSPM観察する際、試料表面 に3から4個の水分子が付着した場合の影響について、興味を持っている。

→ FemAFM_DLVOで、対応可能

μmオーダーでKPFM等の電気的特性を調べるシミュレータが有れば良い。古典電磁 気学の範囲で十分。また、SPMユーザーは、実験結果から、物性値を求めること を望んでいる。物性値をシミュレータに代入してSPM推定画像を得るのと、丁度 逆のことを要求している。このような逆問題に対応できれば、ユーザーのニーズ に適合する。

→ macroKPFM_DLVOで、対応可能

LiqAFMの粘弾性を考慮したtappingモードのシミュレーションには興味を持てる。大気中でカンチレバーを動かし、試料表面に薄い水の被膜が有るような系のシ ミュレーションは興味深い。

→ LiqAFMのtapping機能で、対応可能

DLVO理論のように、電気二重層による斥力を考慮したシミュレーションには期待 が持てる。メゾスコピック系のシミュレーションとして力を入れるべきである。

→ FemAFM_DLVO、macroKPFM_DLVOで、対応可能

どのソルバにおいても、単に、シミュレーションをするのではなく、物理的な量 が分かりやすく計算・導出されるようにした方が望ましい。物理量が絶対的な値 で表示されるように工夫してほしい。

→ 一部、LiqAFMのtapping機能の逆問題で対応可能
すでに、LiqAFMにおいて逆問題ソルバーが完成している
今後は、これをさらに拡張した逆問題ソルバーを開発して対応する予定

たんぱく質などの動的な振る舞いまでシミュレーションできるようになると良い。

様々な材質の微粒子の計測データについて、探針効果を明確にデコンボリュート できるようになるとよい。

→ どのようなソルバーで対応すべきか、方針が未定