

## **Concept of our SPM simulator**

There are various kinds in the Scanning Probe Microscope (SPM), for example, Scanning Tunneling Microscope (STM), Atomic Force Microscope (AFM), Kelvin Probe Force Microscope (KPFM), and so on. We can commonly use these instruments when we measure the structure and properties of sample surfaces over the wide range of scale. Although the SPM was invented a quarter of a century ago, the recent progress of the experimental methods is remarkable, and we have been able to measure the structure, the electronic state, and the mechanical, chemical, electrical/dielectrical, and magnetic properties of the surfaces from the atomic to the nanometer/micrometer scale. Moreover, we can observe not only inorganic materials but also soft materials such as polymer and bio-molecules in liquids, by using the microscopes.

However, it gradually becomes difficult to analyze and understand the measured images and data because the experimental methods also have been elaborated and advanced in order to observe the more complex and finer structures. Therefore, it needs to support the quantitative analyses of the experimental data by the simulations based on the basic theories such as the quantum mechanics.

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Our software has been developed in order to satisfy this need on the cooperation of the world-leading researchers in the theoretical physics, theoretical chemistry, and computer science. We consider that this software can be used not only for the basic research on the nanotechnology but also for the development of the various fields such as catalytic science, electronic devices, surface treatment, fuel cell, polymer, pharmaceutical industry, and nanomedicine. Even if you are not the experts of the theoretical simulations, you can easily operate this software by using its graphical user interface. We can simulate the measurements on the various conditions that the resolution scale is from the atomic to the micro-level one and that the sample is in vacuum, liquid, and air. The experimental methods are progressing and the target of the measurement is enlarging day by day. In order to adapt to the change of the experimental situations in the future, we construct our simulator so as to be easy to extend its function.

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## Functions of our SPM simulator

The SPM simulator consists of the following five solvers:

1. Geometrical mutual AFM simulator: This simulator can provide AFM images quickly based on the geometrical information of a given tip and sample in micro and macro-scale. Moreover, it can predict one of three data (AFM image, a tip-shape, and a sample-shape) from the other two.
2. Finite element method AFM simulator: This simulator can provide AFM images of macro-scale elastic samples including tip-induced-distortion that are not considered in the Geometrical mutual AFM simulator.
3. Soft material liquid AFM simulator: This simulator can provide motion of a macro-scale cantilever in vacuum, air, and liquid, where the cantilever shape can be constructed by users. It will provide AFM images of soft (visco-elastic, bio etc) material samples in cooperation with the Finite element method AFM simulator.
4. Classical force field AFM simulator: This simulator can provide AFM images of the atoms/molecules/nanostructure samples. This includes two type solvers that are CG and MD: CG takes account of the most stable structure for every tip position using the conjugate-gradient optimization, whereas MD considers effects of a finite temperature using the molecular dynamics.
5. Quantum mechanical SPM simulator: This simulator can provide AFM, STM, and KPFM images of atomic-scale samples by calculating the electronic states in accordance with the density-functional based tight-binding (DFTB) method.

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Besides, the SPM simulator has other various functions for efficient operations of the SPM simulator:

- Integrated graphical user interface (GUI): The five solvers of the SPM simulator are integrated by the single GUI. This GUI provides systematic controls for all the solvers.
- A function for building various structures (Modeling Tool): The SPM simulator has additional software for building initial atomic-scale structures. This software provides not only basic structures (like a crystal) but also advanced structures (like a crystal with defects) that you want.
- A function for loading SPM images of various instruments: The SPM simulator can load image files of various SPM instruments directly. This function is useful for comparison between experimental and simulated images.
- A function for tip-shape-prediction: The SPM simulator can predict a tip-shape from the AFM images in accordance with a new method: a combination of the blind reconstruction method and the Geometrical mutual AFM simulator.

We hope that the SPM simulator is useful for not only researchers but also the other persons taking an interest in material science. For this sake, we are going to develop the SPM simulator by adopting users' comments.