Virtual Probe Microscope

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ABSTRACT

Virtual Probe Microscope (VPM) is a tool that has been developed to train users on Atomic Force Microscope (AFM) operation. The benefits from training with VPM include: reduced cost of training and increased transfer of training. The graphical user interface of VPM is laid out similar to common commercial AFM software packages. Along with standard AFM controls, users are given an additional graphical 3D window to view the probe traversing across a surface. Users are also allowed to manipulate probe geometry variable to increase understanding of AFM operation. VPM will be used in a graduate level scanning probe microscopy class in the spring of 2005 at Iowa State University to supplement traditional lab and classroom instruction.

Keywords: atomic force microscope, scanning probe microscope, simulator, simulation

1 INTRODUCTION

With the emergence of every new technology, a demand arises for training scientist and engineers the tools of the new technology. The dawning era of Nanotechnology has created a demand for scientist and engineers to learn many new tools. One of these tools is the Atomic Force Microscope (AFM). An AFM is a type of Scanning Probe Microscope (SPM) primarily used for imaging micro to nano-sized objects. The role of the AFM instrument will become even more important in the decades to come with the shift towards miniaturization.

Training large groups of users to operate an AFM has become a standard procedure with the creation of university courses and industry training sessions. Needless to say, teaching a large group of users can be a very daunting task. The equipment is expensive, the controls are many, and the training is tedious. One of the biggest challenges instructors face is training a large group of novice users on basic AFM operation. Novice users are unfamiliar with equipment and therefore require more attention in a hands-on learning environment. Any instructor will tell you that the combination of hands-on training and repetition is the best way to learn a new skill. However, receiving repetitious hands-on training on an AFM is costly, in terms of time and money.

Parallels of AFM training can be made to aircraft pilot training. Novice pilots do not simply strap into an airplane and take off the run way. Pilots must follow an extensive training program that incorporates both ground-based instruction as well as flight time with an instructor. However, flight time with an instructor is extremely expensive and an instructor can only effectively teach one trainee at a time. To solve these problems, the aviation industry developed flight simulators to provide low cost, multiple user training in a consequence-free environment. Flight simulators decrease the amount of actual flight time that pilots need and increase the amount of positive learned behavior gained from training. Teaching users how to operate an AFM is no different than teaching a pilot how to fly.

A fully interactive AFM training simulator named VPM has been developed to alleviate the problems of training large groups of users on basic AFM operation. VPM is a windows-based simulator that can simultaneously train a room full of users without the need of an actual AFM. Instructors can use this tool to demonstrate the exact same instruction that a trainee would receive in an AFM lab within the confines of a classroom or computer lab. The general mechanics and applications of VPM will be discussed.

2 SIMULATOR COMPONENTS

2.1 Probe-Sample Interaction

An AFM creates an image of a sample by dragging an extremely sharp probe in a raster scanned pattern across a surface. The probe height is sampled at a set interval during the scan creating a 2D array of height values also known as a height map. The height map is then used to create the image of scanned surface.

Theoretically, a perfect AFM image could be achieved using an infinitely sharp probe. In reality, the probe has a measurable geometry. The geometry of the probe will affect the image of the scan as shown in Figure 1. The probe-sample interaction is an important feature for an AFM simulator. Implementing this interaction provides users a useful lesson that a user's scanned images are dependent upon probe geometry.

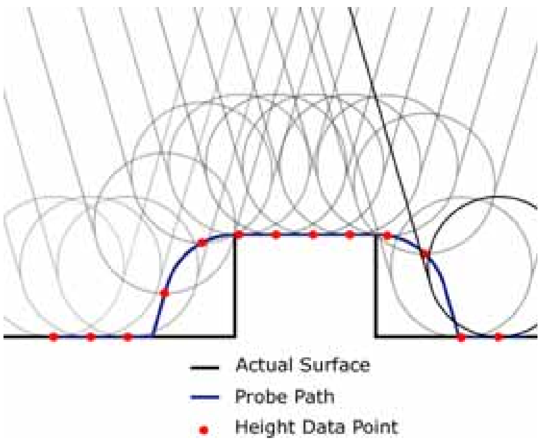

Figure 1: Effect of Probe Geometry on AFM Imaging

Previous AFM simulations have used Mathematical Morphology to simulate the probe-sample interaction [1, 2]. Mathematical morphology uses geometric set theory of shapes to calculate the interaction between two geometries. Using this technique, a surface can be mathematically determined given a probe shape and a surface shape.

VPM takes a different approach to determine the interaction between a probe and the surface, VPM uses an open source collision detection library named OPtimized COllision DEtection (OPCODE) [3]. Collision detection has been primarily used for video game development and virtual assembly simulations, but has been used increasingly more in simulator applications due to advancements in accuracy [4]. Collision detection can be just as accurate as mathematical morphology if used properly. A collision detection algorithm runs on a loop that checks whether two geometries have penetrated at a set interval. If two geometries inner-penetrate further than allowed in between a loop step, the algorithm will attempt to correct the mistake on the next loop forcing the geometries to separate. This separation can cause a jittering effect of the geometries if the interval between two consecutive collision detection loops is not small enough. A comparison study was conducted between the collision detection method and the mathematical morphology method. In the study, a sphere shaped probe scanned a cylindrical feature on a flat surface using the collision detection method [Figure 2]. The results of the study concluded that a collision detection algorithm could be used to obtain a comparable scan to the mathematical morphology method.

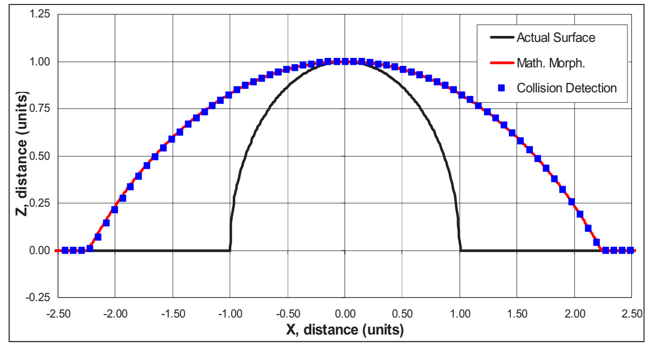

Figure 2: Probe-Sample Interaction Comparison Study

3 SYSTEM DYNAMICS

Tracking the change in height of a probe in a simulated environment is simple. In realty, tracking the height of the probe is extremely complex. An actual AFM uses a combination of a probe mounted cantilever, a piezoelectric crystal, a laser and a photo detector. To accurately replicate a real AFM, a dynamic model must be utilized. The model shown in Figure 3 is used to simulate "contact mode" or "constant force" operation. The VPM user sets a desired force to be applied to the sample, a PID controller adjusts the force applied to the piezoelectric crystal to achieve the desired applied load. When the probe comes across a change in height of the sample, the piezo must react with a change in height. The change in height of the piezo is tracked and stored as the value used to create the image height map.

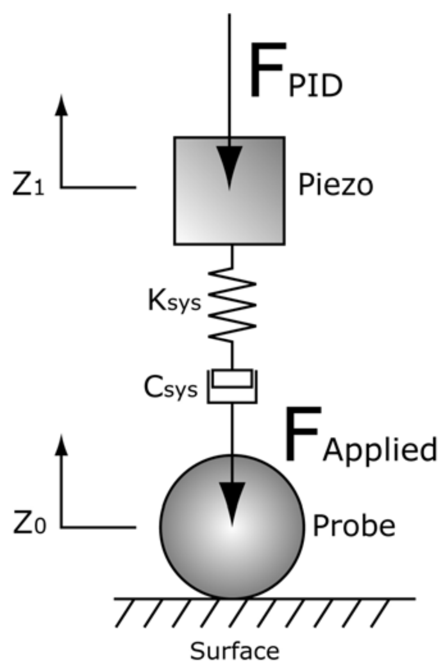

Figure 3: VPM Contact Mode Model

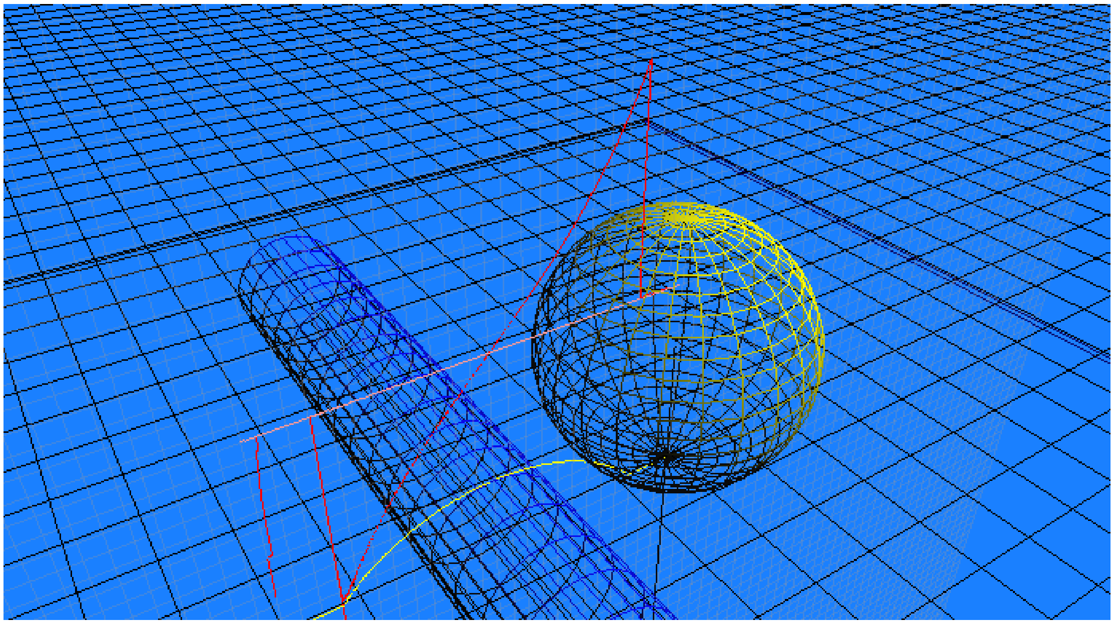

Figure 4: Real time 3D graphical view of a probe and sample

VPM utilizes an open source physics engine named Open Dynamics Engine (ODE) for the dynamic simulation [5]. ODE is a high performance library for simulating rigid body dynamics used in computer games, 3D authoring tools and simulation tools. ODE in conjunction with OPCODE can be used to create systems of joints and geometries to simulate the desired dynamic system.

4 SIMULATOR INTERFACE

The graphical user interface (GUI) for VPM has been created using Microsoft's .NET framework which allows the VPM software to be run on any Windows-capable machine. Furthermore, the Visual Studio development environment allows the simulator to be quickly reconfigured to replicate any desired commercial AFM interface. Replicating the interface that users train for increases the physical fidelity of the simulator. The physical fidelity of a simulator is the extent to which the simulator "looks like" the operational environment [6]. Users who train on a simulator interface similar in layout to the actual interface will generally perform better than if they had trained with a generic interface.

Along with standard AFM controls and windows, several other features were added to the interface to enhance user comprehension and control of the simulator. These features can be found in the following control panels:

- **Simulation Parameters.** This control panel allows users to adjust various parameters of the collision detection and simulation such as simulation time step.
- **Probe Geometry.** Changing probes on an actual AFM involves a steady hand with tweezers. In VPM, users can simply go to the probe geometry control panel and change various dimensions to get achieve a desired probe tip radius.
- **3D Window and Graphics Control.** A real time three-dimensional view has been implemented in addition to the standard 2D top view and line trace view [Figure 4]. The addition of this view is designed to visually aid comprehension of how the AFM system behaves in real time. The controls for this new view are related to view angle and graphics performance.
- **Sample Surface Control.** This control panel allows users to load a desired height map into VPM to be used as a sample surface.

4 VPM IN THE CLASSROOM

In the spring of 2005, a new experimental course entitled ME 561x: Scanning Probe Microscopy will be offered at Iowa State University. The course provides students an introduction to SPM techniques intended for novice users. The format of the course is an 80 minute lecture followed by 50 minutes of laboratory. The lab session will allow students to get a hands-on experience on an AFM. Each lab section has approximately three students sharing time on the atomic force microscope.

To test the usability of VPM, users enrolled in the class will be able to use VPM to assist them in lab activities that include the following:

- Gain optimization
- Contact Mode Operation
- Tip shape effects
- Force curves

At the end of the course, users will be surveyed to assess the student's knowledge of AFM operation. These results will then be compared to data gathered from users who are exclusively trained on the VPM alone. The performance of both groups will be compared to determine the overall effectiveness of the simulation. The results from this study can be used to determine the optimal ratio of time spent on lecture, lab and simulator for AFM training.

5 FUTURE WORK

Virtual Probe Microscope is still in its infancy. Further work will involve adding complexity to the simulator, increasing VPM's functional fidelity. Functional fidelity is similar to the concept of Physical Fidelity discussed in the previous section. Functional fidelity is the degree to which the simulator "acts like" the operational environment - does the simulator produce the same response as the actual instrument when given the same input [6]? Increasing the functional fidelity of a simulator will generally increase the amount of positive learned behavior that can be transferred from the training simulator to the operational environment.
Areas of future work include the following:

- **Contact Mechanics.** To accurately simulate force curves on an AFM, adhesive forces must be employed. Users will be allowed to select which contact theory to use in the simulation: Hertzian, DMT or JKR.

- **Advanced Probe Geometry.** Users will be able to load probe geometry from file, or construct non sphere-swept cone geometry. Non-symmetrical geometry can be used to demonstrate tip characterization.

- **Deformable Surfaces**. Because VPM uses a rigid body dynamics engine, the tool is limited to scanning materials with an infinitely hard surface. A deformable surface could be implemented to simulate the scanning of soft or biological materials.

- **Lateral Force Mode**. This AFM operation mode allows users to calculate friction on surfaces independent of variation of sample topology. Many courses cover this mode and it would benefit VPM users to be able to operate in this mode.

6 CONCLUSION

Virtual Probe Microscope has been successfully developed as an AFM simulator to train a large group of users on basic AFM operation. Advantages of using the simulator for training include a reduction in cost of training, reduction in time of training, and an increase in hands-on learning. Additional feature not found on standard AFM interfaces have been implemented to increases transfer of learning from simulator to operational environment. Future usability studies on VPM will provide insight into the best possible use of the simulator.

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