Title:
Simulating the Approach-retract Phenomenon of AFM in Virtual Environment with Haptic Interface

Authors:
Ke Liu, kliu@student.pvamu.edu, Prairie View A&M University
Xiaobo Peng, xipeng@pvamu.edu, Prairie View A&M University

Keywords:
Virtual Environment, Haptic Interface, AFM, Approach-retract Phenomenon

DOI: 10.14733/cadconfP.2015.89-93

Introduction:

Nanotechnology is an exciting and growing area, which includes diverse fields of science such as physics, biology, surface science, microfabrication, etc. The Atomic Force Microscope (AFM) is a crucial technique to study nanotechnology. It can be used to study cell stiffness for potential disease diagnosis. The nanoscratching lithography can be implemented by AFM. However, AFM technique lacks of real-time visual feedback, because only static scanning images are provided in real AFMs. Normally, the cost and the maintenance of the AFM are expensive. The preparation of AFM is also challenging for an instructor who is not an expert in nanotechnology. The experience would also be limited for students to use such kind of tool, since professional operators are necessary to make the AFM ready. The nanoscale phenomena are difficult for researchers and students to understand and conceptualize. It would be beneficial to develop an AFM Virtual Reality (VR) system which could help people understand the nanoscale phenomenon through tools in macro world. The haptics can express force variations intuitively.

Main Idea:

The goal of our work is to investigate how virtual reality technique can be used to help people understand nanoscale phenomenon. A virtual environment with haptic interface was developed to simulate the Approach-retract (AR) phenomenon of AFM. Five research tasks were carried out in this work: (1) Constructing the graphic display of the virtual scene of the nanoscale sample surface and AFM probe. In our case, the shape of silicon nitride tip is employed and the sample surface shows the arrangement of atoms. (2) Researching the force-displacement curves between tip and sample surface. In this project, the force-displacement curves were defined by contact line, “jump to contact” distance [5], and “jump off contact” force [4]. (3) Developing the haptic force models to simulate the real interaction between the AFM probe and sample surface. (4) Integrating various force models into the system to simulate the interaction between the AFM probe and different characteristics of samples (mica, gold, silicon nitride). In this research, the force models were implemented with different Hamaker constants and surface energy from various material attributes. (5) Evaluating the effectiveness and fidelity of the AFM virtual reality simulation. Compared to other researches, this simulation provides more accurate force models of AR phenomenon. Multiple sample material choices are available as well.

The developed VR simulation is intuitive and no training is needed. It can provide users a 3D view of the manipulation scene in real time. The interactivity provided by haptic interface helps users better understand nanoscale forces and objects. It increases students’ perception of nanoscale phenomenon. Compared to operating a real AFM, the expense of virtual reality simulation is cheaper and the chances to access to the tool is unconstrained. The simulation allows people touch the unfamiliar nano-world through the familiar macro world. The simulation can be used to teach students or train professional researchers.

Development of force functions

The force-displacement curves as shown in Fig. 1. can be used to describe the Approach-retract (AR) phenomenon of AFM. The curves are plots of tip-sample interaction forces vs displacement of piezoelectric scanner, Z. Generally, the force-displacement curves can be divided into three regions: the contact region, the non-contact region and the zero line. In Fig. 1., zero line is presented as AC which means the cantilever is far from the sample surface and there is no deflection on it. The non-contact region is represented as CD and BF which are described as fast force variations. The line CD represents the “jump to contact” line. The line BF represents “jump off contact” line. The maximum value of the attractive force, F_{attr} , equals the pull-on force. The maximum value of adhesion force, F_{ad} , equals the pull-off force. Point C and point B represent the displacement where the “jump to contact” variation and “jump off contact” variation happen respectively. Z_{jtc} represents the "jump to contact" displacement. Z_{joc} represents the "jump off contact" displacement. In order to develop the force functions of AR phenomenon, Z_{jtc} , $k^{'}$, and F_{ad} are the key values needed to be found.

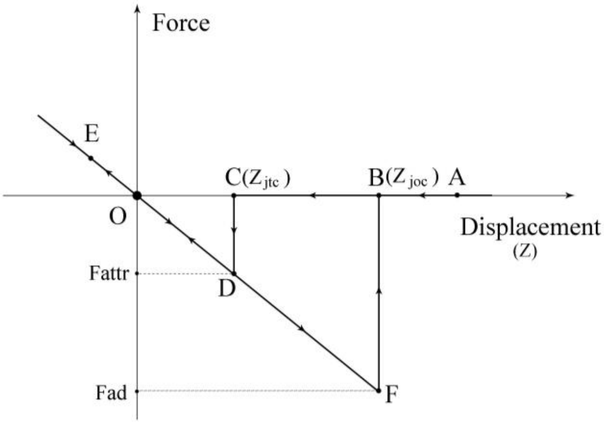


Fig. 1: Three regions of the force-displacement curves.

The contact force can be defined by [3]:

$$F = \frac{k_c k_s}{k_c + k_s} Z = k^{'} Z \tag{1}$$

where k_c is the elastic constant of cantilever, k_s is the elastic constant of sample surface, and δ_c is the cantilever deflection. Eqn. (1) exactly explains the contact line which is shown as EF in Fig.1. Literatures have shown that generally the sample stiffness is much bigger than cantilever's stiffness [7]. Therefore, in this research, it is assumed that $k_s >> k_c$, then $k^{'} \cong k_c$.

According to Hao et al.’s work [5], the cantilever-sample system can be described by means of potential. Z_{jtc} could be obtained:

$$Z_{jtc} = D_{attr} + \alpha(\delta_c)_{attr} \tag{2}$$

$$(\delta_c)_{attr} = \frac{1}{2}\sqrt[3]{\frac{A_H R}{3\alpha^2 k_c}} \tag{3}$$

$$D_{attr} = \sqrt[3]{\frac{\alpha A_H R}{3k_c}} \tag{4}$$

$$\alpha = 1 + \frac{k_c}{k_s} \tag{5}$$

where $(\delta_c)_{attr}$ is the cantilever deflection at which "jump to contact" occurs. D_{attr} is the distance between the tip and sample surface when the tip "jump to contact." The A_H stands for the Hamaker constant and R is the radius of the tip.

The adhesion force F_{ad}, which is also called pull-off force, was calculated based on Derjaguin-Müller-Toporov theory [4]. The adhesion force is:

$$F_{ad} = -2\pi R W_{ad} \tag{6}$$

where R is the tip radius and W_{ad} is adhesion work per unit area at contact. The work of adhesion is usually replaced by twice the surface energy of the solid [1]: $W_{ad} = 2\sqrt{\gamma_s \gamma_t}$. γ_s represents sample surface energy and γ_t stands for tip surface energy.

Programs of Simulation

The simulation of the AR phenomenon of AFM was developed using software Vizard. The simulation was displayed in the PowerWall Virtual Environment. The haptic device Phantom Omni was used to track the cantilever of the AFM. The most critical part of the simulation is to apply forces to the reflect different regions of force-displacement curves. When "current position of the Phantom>= Z_{joc} ", the tip is far away from the sample surface. No force is applied between cantilever tip and sample surface. This region is represented as AB in Fig. 1. When " Z_{jtc} <=current position of the Phantom< Z_{joc} ", two cases may occur. The corresponding regions in Fig. 1 are BC and DF. If the tip is being retracted from the sample surface (current position>=previous position), the spring force should be assigned. When the tip is approaching the sample surface (current position<previous position), the spring force should be removed. When "0<current position of the Phantom< Z_{jtc} ", the tip is in contact with the sample surface. This region is shown as DO in Fig. 1. The spring force should be applied during this procedure. The cantilever beam bends downward when "-deformation<=current position<=0". The spring force is still exist in this process. This region is presented as OE in Fig. 1.

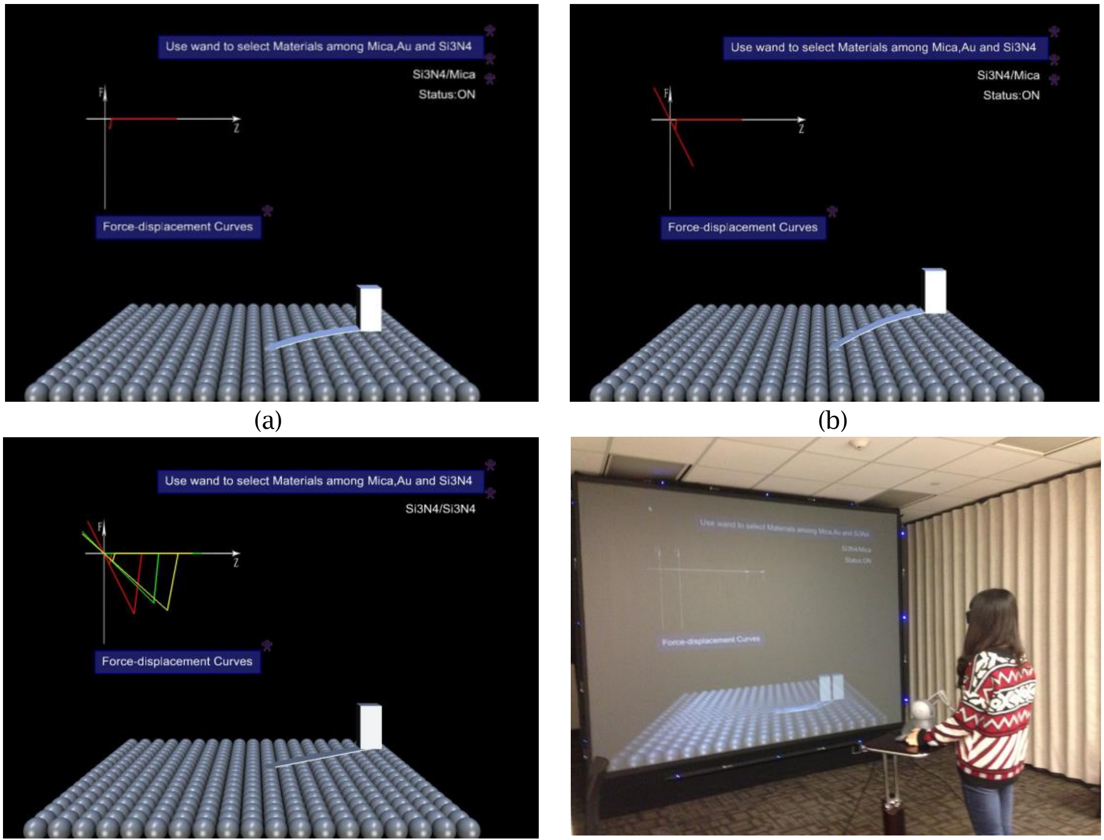
Results and Verifications

The AFM AR phenomenon simulation simulates the interaction of the tip with three different sample materials, including mica, gold, and silicon nitride. According to different sample attributes (mainly Hamaker constant and tip-sample energy), the variables mentioned above were applied in the simulation.

The AFM simulation can be operated in the following steps. Firstly, the user can use the wand to select a sample material from mica, gold or silicon nitride. The material information of the cantilever tip and the sample is displayed in the graphic window. The cantilever is tracked by the Phantom in the simulation. Secondly, the user needs to hold the pen of Phantom and lift it to its highest threshold. After the Turn-On button on the Phantom is pressed, the force output are enabled. Thirdly, the operator has to move the pen for one cycle. One cycle in Approach-retract phenomenon refers to move the cantilever downward until the cantilever beam bends and then move it upward until there is no atomic interaction force anymore. When the tip is approaching the sample surface, the force-displacement curves will be displayed as zero line instantly. The "jump to contact" occurs when the tip reaches the "jump to contact" displacement. At this moment, the user can feel the sudden attractive force as shown in Fig. 2(a). The operator can still feel the spring force while moving downward further. When the tip is in contact with the sample surface, the cantilever beam bends if the user keep moving downward. During the retracting process, the spring force exists until the tip reaches the "jump off contact" displacement as shown in Fig. 2(b). After that, the user feels a sudden release and there is no interaction force between tip and sample surface anymore. The operator could press the Turn-Off button at any time during the process to disable the force output. Fig. 2(c) shows the complete force-displacement of three sample materials. Fig. 2(d) shows a student is using the AFM simulation.

In order to examine the accuracy of the force model developed in this work, the calculated data were compared to physical experimental data. The calculated data were obtained based on force functions developed above. The experimental data were obtained from others' work [2, 3, 6]. The data generated from the simulation were also compared to physical experimental data. The data are presented in Tab. 1. When the calculated data were compared to experimental data of mica, the calculated attractive force is 0.54% less than the experimental attractive force and the calculated adhesion force is 0.06% less than the experimental attractive force. Compared to the experimental data of mica, the simulated attractive force is 4.09% less than experimental attractive force and simulated adhesion force is 0.09% less than experimental adhesion force. The data from other two sub-simulations can also be found in Tab. 1.

Twenty students were invited to use and evaluate the AFM simulation. Students' understanding of the Approach-retract phenomenon were analyzed by implementing a survey. The survey showed that the students' perceptions of nanoscale phenomenon have been improved after using the simulation. The survey results also indicated that the haptic feedback is more helpful than the visual feedback in the sensory feedback of AFM simulation. All of the students believed that the virtual reality simulation would play an important role in understanding nanoscale phenomenon. The AFM simulation also increased their interest in nanoscale phenomenon a lot.



(a) (b)

(c) (d)

Fig. 2: Snapshots of simulation: (a) sudden attractive force, (b) adhesion force, (c) force-displacement curves of three sample materials, (d) a user in operation.

Mica				
Data type	F_{attr} (nN)	Difference (Compared to experiment)	F_{ad} (nN)	Difference (Compared to experiment)
Calculation	0.2387	-0.54%	1.3992	-0.06%
Simulation	0.23019	-4.09%	1.39877	-0.09%
Experiment	0.24	_	1.4	_
Gold				
Calculation	0.4071	1.78%	9.9946	-0.05%
Simulation	0.39962	-0.10%	9.99359	-0.06%
Experiment	0.4	_	10	_
Silicon Nitride				
Calculation	0.09	-10%	0.5997	-0.05%
Simulation	0.08815	-11.85%	0.58551	-2.42%
Experiment	0.1	_	0.6	_

Tab. 1: Data comparisons in three sub-simulations.

Conclusions:

The paper describes the virtual environment with haptic interface developed for the simulation of AFM manipulation. The van der Waals force was employed for the modeling of “jump to contact” displacement. Adhesion force was developed from Derjaguin-Müller-Toporov theory for contact region. The haptic force models were established for simulation. Simulations based on different attributes of various materials (mica, gold, and silicon nitride) were developed. The data output from the simulation were compared to physical experimental data to verify the accuracy of the simulation. The results showed that the simulation provides a relatively accurate insight into the mechanism of an AFM based nanoscale manipulation. Survey results showed that the simulations are interactive and intuitive for students since the users are able to obtain real-time visual and haptic feedback.

Acknowledgement:

This research is supported by National Science Foundation award HRD-1137578.

References:

[1] Butt, H. J.; Cappella, B.; and Kappl, M.: Force measurements with the atomic force microscope: Technique, interpretation and applications, Surface Science Reports, 59(1), 2005, 1-152. http://dx.doi.org/10.1016/j.surfrep.2005.08.003

[2] Cappella, B.; Baschieri, P.; Frediani, C.; Miccoli, P.; Ascoli, C.: Force-distance curves by AFM, Engineering in Medicine and Biology Magazine, IEEE, 16(2), 1997, 58-65. http://dx.doi.org/10.1109/51.582177

[3] Cappella, B.; Giovanni D.: Force-distance curves by atomic force microscopy, Surface Science Reports, 34(1), 1999, 1-104. http://dx.doi.org/10.1016/S0167-5729(99)00003-5

[4] Derjaguin, B. V.; Muller, V. M.; Toporov, Y. P.: Effect of contact deformations on the adhesion of particles, Journal of Colloid and Interface Science, 53(2), 1975, 314-326. http://dx.doi.org/10.1016/0021-9797(75)90018-1

[5] Hao, H. W.; Baro, A. M.; Saenz, J. J.: Electrostatic and contact forces in force microscopy, Journal of Vacuum Science & Technology B, 9(2), 1991, 1323-1328. http://dx.doi.org/10.1116/1.585188

[6] Meurk, A.; Luckham, P. F.; Bergström, L.: Direct measurement of repulsive and attractive van der Waals forces between inorganic materials, Langmuir, 13(14), 1997, 3896-3899. http://dx.doi.org/10.1021/la9610967

[7] Pawluk, D.; Taylor, C.; Hoffman, M.; McClintock, M.: Development of a Nanoscale Virtual Environment Haptic Interface for Teaching Nanotechnology to Individuals who are Visually Impaired, American Society for Engineering Education. American Society for Engineering Education, 2009.