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# Simulating the approach-retract phenomenon of AFM in virtual environment with haptic interface

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#### ABSTRACT

Atomic Force Microscope (AFM) is a crucial technique to study nanotechnology. The virtual reality simulation presented in this paper could be used to teach students or train professional researchers on approach-retract (AR) phenomenon. Based on different Hamaker constants and surface energies from various sample materials (mica, gold, and silicon nitride), various analytical force models of AR phenomenon were developed. The force models were simulated in the virtual environment using haptic device. Students were asked to complete surveys to examine the role of this simulation in the understanding of AFM. Results showed that students' perceptions of nanoscale phenomenon have been improved after using the simulation.

#### KEYWORDS

Virtual environment; haptic interface; AFM; approach-retract phenomenon

# 1. 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 high-resolution type of scanning probe microscope. It is one of the foremost tools for people to image, measure, and manipulate materials in nanoscale. With AFM the operators use a cantilever beam with a sharp tip at its end to scan sample surfaces. Typically, the cantilever consists of silicon or silicon nitride with a tip radius of curvature in the scale of nanometer. The motion of the cantilever beam is controlled by the feedback loop and piezoelectric scanner. The feedback loop is a mechanism which could protect the tip from colliding with the surface. The piezoelectric scanner is used to move the sample in x, y, and z directions. The deflection of the cantilever is measured with a laser spot which is reflected from the top of the cantilever into the photodetector. According to its application, the AFM could be operated in a number of modes: static modes (contact mode) and dynamic models (non-contact mode or tapping mode).

The Atomic Force Microscope (AFM) has wide applications in nanotechnology. The AFM can be used as an effective tool in the nano-fabrication and nano-assembly for fabricating nano-scale devices and nano-structures. It can be used to study cell stiffness for potential disease diagnosis. The nanoscratching lithography can be implemented by AFM as well. However, AFM technique lacks of real-time visual feedback during the manipulation process, because only static scanning images are provided in real AFMs. The cost and the maintenance of the AFM are expensive. The preparation of AFM is also challenging for users. Professional operators are necessary to make the AFM ready. The nanoscale phenomena are difficult for researchers and students to understand and conceptualize.

Literatures have shown that it is beneficial to use Virtual Reality (VR) simulation to improve people's understanding of nanoscale phenomena [6], [9], [11], [12], [14]. Virtual Reality (VR) is referred to the technology which can be used to simulate the physical real world environment. People can interact with the computer simulated environment through sight, sound, touch, etc. The haptics is defined as assigning forces to the operational point of a haptic interface based on the information of the virtual environment [13]. Integrating the haptic device in the AFM related VR system allows people to gain an intuitive sense of force interaction. The haptics can express force variations intuitively.

The objective of this work is to develop various analytical force models to simulate the interaction between the AFM probe and different material samples. With such functions, the user can identify not only the topology of the sample surface but also the material characteristics of the sample. The ultimate goal of the research is to use virtual reality system to simulate the AFM based nanomanipulation. Such a system can be used to teach students or train professional researchers the AFM based nano-fabrication and nano-assembly in the future.

The paper presents the development of the virtual environment with haptic interface to simulate the Approach-retract (AR) phenomena of AFM. The AR phenomena is referred to the mechanical behavior of the AFM probe when it touches a sample surface in the vertical direction. In this work, the virtual scene of the nanoscale sample surface and AFM probe were constructed and displayed in 3D. The force-displacement curves between tip and sample surface were researched. The haptic force models were developed and integrated into the system to simulate the real interaction between the AFM probe and different sample materials. Compared to others' research, this simulation provides more accurate force models of AR phenomenon. Multiple sample material choices are available as well.

The AFM simulation presented in this paper has many benefits. The 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 are unconstrained. The simulation allows people touch the unfamiliar nanoworld through the familiar macro world. This virtual reality system developed in the project can be used to teach students or train professional researchers.

# 2. Related work

Haptic devices have been used in AFM related simulations by researchers. In Sitti and Hashimoto's work, a teleoperated nanoscale touching system was developed [14]. Nanocontact mechanics models were introduced. The simulation was realized through a 1 DOF haptic device and force-reflecting servo type scaled teleoperation controller. Researchers found out that visual feedback alone cannot provide enough information since it may include many source of errors (such as positioning drift, nonlinearities, noises, etc.) As a result, real-time force feedback is one of the promising solutions for compensating these errors. The simulation results showed that the proposed system allowed operators to feel the scaled nanoscale adhesion forces repeatedly on operators' fingers. Also, the system enabled operators to feel the nanoscale surface topography as well as contact/noncontact nanoforce feedback.

Millet et al. [11] developed a pedagogical tool using haptic feedback and two graphic representations to simulate the approach-retract cycle of an AFM probe. The two graphic representations included a virtual AFM cantilever and a virtual magnet-spring system whose haptic behavior is analog. Both methods were appreciated and had an influence on students' understanding. Also, the magnet-spring analog appeared to be a good alternative for an introductory course of AFM. The result showed that it was more efficient for participants without prior knowledge to understand the approach-retract phenomena of an AFM probe with both haptic feedback and visual analogies.

In Pawluk et al.'s study [12], a force feedback device called Novint Falcon was used as a cantilever tip of an AFM to help students easily switch between experiencing the macro scale and nanoscale for comparison purpose. As a result, the learning process could be facilitated by allowing students to learn nanoscale from a more familiar analog. There were two modules in their simulation. The first module let students understand the concept of scale between the two worlds and how they are a continuum. The second module allowed students to feel the flick-to-contact instability calculated based on van der Waals force. By making the adhesion 100 times greater than the flick-to-contact force, students could also feel the approach-retract hysteresis.

Li et al. implemented an augmented reality system which enables the real-time visual feedback of nanomanipulation by locally updating AFM image [9]. This system allowed operators to feel the force interactions during nanomanipulation through a haptic device (PHAN-TOM). At the same time, the real-time changes of the nano environment were provided as well. It was shown that nanopatterns can be accurately created and the nanoparticles can be easily manipulated on the sample surface using the newly developed augmented reality system without the need of a new image scan. This augmented reality system was capable of the nanolithography and manipulation of nano-particles.

Fok et al. described the development of a haptic interface for AFM nanomanipulation [6]. The whole system enabled operators to touch the sample surface while manipulating with the cantilever tip in AFM. The Lennard-Jones potential was employed for modeling tipsample interaction force while they are in contact. The JKR theory is applied for indentation and adhesion force. The motion behaviors of the AFM cantilever and relations between the applied force and depth of indentation were analyzed. The whole system was aimed at offering a virtual reality interface to display topography of surface and help operators predict the results of the manipulation.

Most of the previous work mentioned above focused on examining the effectiveness of using haptic interface to enhance the users' perception and learning of nanoscale phenomena in AFM. Few researches have proposed analytical haptic force models which could be employed in the AFM related simulations. In our work, the analytical haptic force models were defined as functions of material properties. The system can simulate the interaction between the AFM probe and different material samples. The accuracy of the force models were verified by comparing the calculated and simulated data with physical experimental data.

# 3. Development of force functions of AR phenomenon in AFM

#### 3.1. AR phenomenon in AFM

The AFM is a scanning probe microscope, which can be used to collect an image based on the interaction between the sample and tip. The sample is scanned by a tip, which is at the end of the cantilever beam as shown in Fig. 1. Because of its microscale dimensions, the cantilever beam is sensitive enough to bend due to small forces (mainly van der Waals force is approximately 0.3nN) [12]. The force between the sample surface and the tip is measured by monitoring the deflection of the cantilever. A topographic image of the sample can be obtained by plotting the deflection of the cantilever versus the displacement of the sample position. In actual AFM, the probe never moves. It is the sample that is moved in the X, Y, Z directions by a piezoelectric scanner. In this research, relative move between sample and tip was employed to realize the simulation. In the AFM simulation, the sample would be kept still. The operators are able to sense the force while moving the tip.



Figure 1. Schematic of an Atomic Force Microscope.

Fig. 2. shows a contact AFM force versus relative positions (displacement) of the tip and sample surface. When the tip is approaching the sample surface from far away (from A to C in Fig. 2.), the attractive forces is zero at this time. At point C, the tip is pulled onto the sample surface due to the sudden attractive force. This is the first fast force variation of force-displacement curves. As the tip presses into the sample surface (from D to E), cantilever is pushed up due to the contact mechanics. The force increases during this process. As the tip retracts from E to F, the force decreases. The tip continues retracting until it reaches a pull-off force at point F. The tip breaks free from surface attraction (from F to B). This is the second fast force variation of force-displacement curve. Line BA explains no contact between tip and sample surface anymore. The adhesion force encountered during retraction is significantly larger than the attractive force encountered during approach. This phenomenon is considered as the Approach-retract (AR) phenomenon.



Figure 2. The force-displacement curves in AFM.

# 3.2. Force functions of AR phenomenon

The force-displacement curves as illustrated in Fig. 2 are plots of tip-sample interaction forces vs displacement of piezoelectric scanner (Z). The force-displacement curves can be divided into three regions: the zero line, the contact region, and the non-contact region. In Fig. 2 zero line is presented as AC which means the cantilever is far from the sample surface and there is no deflection on it. The contact region is represented by line EF where the tip is in contact with the sample surface. 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.

The contact line EF can be defined by [4]:

$$F = \frac{k_c k_s}{k_c + k_s} Z = k' Z \tag{3.1}$$

where  $k_c$  is the elastic constant of cantilever,  $k_s$  is the elastic constant of sample surface. Literatures have shown that generally the sample stiffness is much bigger than cantilever's stiffness [12]. Therefore, in this research, it is assumed that  $k_s \gg k_c$ , then  $k' \cong k_c$ .

The adhesion force  $F_{ad}$  was calculated based on Derjaguin-Müller-Toporov theory [5]. The adhesion force is:

$$F_{ad} = -2\pi R W_{ad} \tag{3.2}$$

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 [2]:

$$W_{ad} = 2\sqrt{\gamma_s \gamma_t} \tag{3.3}$$

where  $\gamma_s$  represents sample surface energy and  $\gamma_t$  stands for tip surface energy. The  $F_{ad}$  could be calculated based on Eqns. (3.2) and (3.3):

$$F_{ad} = -4\pi R \sqrt{\gamma_s \gamma_t} \tag{3.4}$$

The displacement Z as shown in Fig. 3. can be represented as:

$$Z = D + (\delta_c + \delta_s) \tag{3.5}$$

where D is the distance between the tip and the sample surface,  $\delta_c$  is the cantilever deflection and  $\delta_s$  is the sample deformation.



Figure 3. The tip-sample system.

According to Hao et al.'s work [7], the cantileversample system can be described by means of potential. The "jump to contact"  $Z_{jtc}$  could be obtained:

$$Z_{jtc} = D_{attr} + \alpha(\delta_c)_{attr}$$
(3.6)

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".  $\alpha$  is defined by

$$\alpha = 1 + \frac{k_c}{k_s} \tag{3.7}$$

 $D_{attr}$  and  $(\delta_c)_{attr}$  can be found by:

$$D_{attr} = \sqrt[3]{\frac{\alpha A_H R}{3k_c}} \tag{3.8}$$

$$(\delta_c)_{attr} = \frac{1}{2} \sqrt[3]{\frac{A_H R}{3\alpha^2 k_c}}$$
(3.9)

where  $A_H$  stands for the Hamaker constant and R is the radius of the tip. Therefore,  $F_{attr}$  can be calculated by

$$F_{attr} = k' \times Z_{jtc} \tag{3.10}$$

#### 3.3. Data used in simulation

Three different sample materials were selected to study the AR phenomenon in the simulation, including mica, gold, and silicon nitride ( $Si_3N_4$ ). The data of the three materials are listed in Tab. 1. The material of the tip is  $Si_3N_4$ . The tip radius R was set to be 50 nm. Typically, the spring constant of the cantilever is defined between 0.1N/m and 0.3 N/m [12]. In this work, the slope of the force-displacement curves is set to be  $k' \cong$  $k_c = 0.1N/m$  when the sample material is mica and gold,  $k' \cong k_c = 0.036N/m$  when the sample material is silicon nitride. It is assumed that  $k_s \gg k_c$ , so  $\alpha = 1 + \frac{k_c}{k_s} \cong 1$ . The Hamaker constant  $A_H$  of  $Si_3N_4$  and Mica with water medium is calculated by Bergström [1]. The  $A_H$  of  $Si_3N_4$ 

 Table 1. Data used in AFM simulation.

Тір	Si <sub>3</sub> N <sub>4</sub>	Si <sub>3</sub> N <sub>4</sub>	Si <sub>3</sub> N <sub>4</sub>
Sample	Mica	Gold	Si <sub>3</sub> N <sub>4</sub>
Medium	Water	Water	Diiodomethane
R(nm)	50	50	50
<i>k</i> ′ (N/m)	0.1	0.1	0.036
$A_{H}(\times 10^{-20}J)$	2.45	12	1
D <sub>attr</sub> (nm)	0.799	1.357	1.667
$(\delta_c)_{attr}(nm)$	1.598	2.714	0.834
Z <sub>itc</sub> (nm)	2.397	4.071	2.501
F <sub>attr</sub> (nN)	0.240	0.407	0.090
$\sqrt{\gamma_s \gamma_t} (mJ/m^2)$	2.228	15.915	0.955
$F_{ad}(nN)$	1.3992	9.9946	0.5997
Z <sub>joc</sub> (nm)	13.992	99.946	16.658



Figure 4. Program flow chart of the AFM simulation.

and  $Si_3N_4$  with medium diiodomethane is measured by Meurk et al. [10]. The  $A_H$  between  $Si_3N_4$  and gold could not be found. Instead, the  $A_H$  between  $SiO_2$  and gold with medium water was adopted form Hillier et al.'s work [8]. The data of surface energy  $\sqrt{\gamma_s\gamma_t}$  are adopted from the works of Cappella et al. [3] and Meurk et al. [10] respectively. The values of  $Z_{jtc}$ ,  $F_{attr}$ ,  $Z_{joc}$ , and  $F_{ad}$  are calculated using the equations derived in Section 3.2.

## 4. Development of simulation

The simulation of the AR phenomenon in AFM was implemented and tested on a Microsoft Windows XP workstation with a Xeon 2.4G Hz CPU, 6GB RAM, and NVidia Quadro FX5800 graphics card. The simulation 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 POWERWALL is a single, flat, large-scale (10 ft by 7.5 ft) stereoscopic screen illuminated from the rear by a video projector. The Wand was used an input device which allows the user to manipulate the 3D scene in the virtual environment.

The program flow chart of the simulation is shown in Fig. 4. The sample material has to be selected first. Then the haptics needs to be initiated and enabled. The user moves the tip by controlling the PHANTOM. Based on the position data of the PHANTOM, the tip-sample interaction force is calculated. The calculated force is then applied to the haptic device so that the user will feel the force. The force-displacement curves are drawn with position and force data in real-time.

The most critical part of the simulation is to apply forces to reflect the different regions of forcedisplacement curves as shown in Fig. 2. When "current position of the PHANTOM  $> = Z_{joc}$ ", the tip is far away from the sample surface. The force between cantilever tip and sample surface is zero. No force is applied. This region is represented as AB in Fig. 2. When " $Z_{jtc} < =$  current position of PHANTOM  $< Z_{joc}$ ", there could be two cases. The corresponding regions in Fig. 2. are BC and DF. If (current position of the PHAN-TOM > = previous position of PHANTOM), the tip is being retracted from the sample surface (represented as DF in Fig. 2.). The spring force F = k'Z is applied to the user through PHANTOM. If (current position < previous position), the tip is approaching the sample surface (represented as BC in Fig. 2.). No force is applied. When "current position of the PHAN-TOM <  $Z_{jtc}$ ", the tip is in contact with the sample surface. This region is shown as DE in Fig. 2. The spring force F = k'Zshould be applied during this procedure.

#### 5. 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 described in Section 3.3 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 the PHANTOM and lift it to its highest threshold. After the Turn-On button on the PHANTOM is pressed, the force output is 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. 5(a). When the operator continues moving the tip downward, the cantilever beam bends downward. The user can still feel the spring force as shown in Fig. 5 (b). During the retracting process, the spring force exists until the tip reaches the "jump off contact" displacement as shown in Fig. 5(c). After that, the user feels a sudden release and there is



**Figure 5.** Screenshots of AFM simulation: (a) sudden attractive force, (b) cantilever bends, (c) sudden adhesion force, (d) zero interaction force, (e) force-displacement curves of three sample materials, and (f) a user in operation.

no interaction force between tip and sample surface anymore as shown in Fig. 5(d). Fig. 5(e). shows the complete force-displacement curves of three sample materials. Fig. 5(f). shows a student is using the AFM simulation.

In order to examine the accuracy of the force models developed in this work, the calculated data were compared to physical experimental data. The calculated data were obtained based on force functions developed in Section 3.2. The experimental data were obtained from others' work [3], [10]. The data generated from the simulation were also compared to physical experimental data. The data are presented in Tab. 2. In most cases, the calculated data and simulation data are in good agreement with the experimental data with the differences ranging

Table 2. Data comparisons in three sub-simulations.

Data type	F <sub>attr</sub> (nN)	Difference (Compared to experiment)	F <sub>ad</sub> (nN)	Difference (Compared to experiment)
Mica				
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	-

from -4.09% to 1.78%. Relative large discrepancies were found in attractive force for sample material silicon nitride. The calculated attractive force is 10% smaller than the experimental attractive force. The simulation attractive force is 11.85% less than experimental attractive force. The discrepancies could be attributed to the difficulty and uncertainty when measuring the forces in experiments using AFM. The presence of different types of forces, the difficulty of eliminating contaminants, and the lack of knowledge of the tip shape make the measurement problematic [4]. Therefore, the discrepancies are considered acceptable.

Twenty students were invited to use and evaluate the AFM simulation. Students' understanding of the Approach-retract phenomenon was analyzed by implementing a survey. The survey includes 8 questions. The survey results are shown in Tab. 3. Students rated their responses on a scale of four: 4 indicating a response of "A great deal", 3 indicating a response of "A lot", 2 indicating a response of "Somewhat", 1 indicating a response of "A little", and 0 indicating a response of "Not at all". 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.

Table 3. AFM simulation survey results.

Survey questions	Mean	SD
How much did the AFM simulation add to your understanding of AFM manipulation?	3.50	0.61
How much did the AFM simulation add to your understanding of Approach-retract phenomenon?	3.45	0.69
How much did the AFM simulation add to your understanding of Force-displacement curves?	3.50	0.61
How much did the haptic interface help you understand those concepts listed above?	3.35	0.81
How much did the 3D graphics help you understand those concepts listed above?	3.15	0.75
How interesting was the AFM simulations?	3.80	0.41
Do you believe other virtual reality simulations would be helpful in increasing your understanding of nanoscale phenomenon?	4.00	0.00
How much did the AFM simulation increase your interest in nanoscale phenomenon?	3.25	0.79

# 6. Conclusions

This paper describes the virtual environment with haptic interface developed for the 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 developed for the simulations. Simulations based on different attributes of various materials (mica, gold, and silicon nitride) were implemented. The data output from the simulation were compared to physical experimental data to verify the accuracy of the simulation. The results show that the simulation provides a relatively accurate insight into the mechanism of an AFM based nanoscale manipulation. The real-time visual feedback through POWERWALL system and haptic feedback provided by haptic device are important for people to learn nanoscale phenomenon intuitively. The simulations are interactive and intuitive for students since the users are able to obtain real-time visual and haptic feedback.

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