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An Educational Simulation for Understanding Atomic Force Microscopy Image Artifacts

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Dr. John Liu is the Principal Investigator of the MIT Learning Engineering and Practice (LEAP) Group, which applies design principles to solving challenges to better meet the increasing demand for STEM skills in tomorrow's workforce. He is a Lecturer in MIT's Mechanical Engineering department and MITx Digital Learning Lab Scientist. He leads education and workforce development efforts for MIT's new initiative: Manufacturing@MIT. He was the Director of the Principles of Manufacturing MicroMasters program, an online certificate program that has now enrolled over 180,000 learners across the globe. Dr. Liu's work includes engineering education, mixed reality and haptic experiences, workforce solutions to address the nation-wide manufacturing skills need, open-ended assessments for scalable education settings, and instructional design theory for massively open online courses. He received Best Paper Awards at the American Society Engineering Education (ASEE) in 2020. Dr. Liu earned his B.S. in Applied Physics from Caltech and S.M. and Ph.D. in Mechanical Engineering from MIT, under an MIT-SUTD fellowship and NSF Graduate Research Fellowship.

An Educational Simulation for Understanding Atomic Force Microscopy Image Artifacts

Abstract

The atomic force microscope (AFM) is a fundamental imaging tool used to visualize minute features, often on the scale of fractions of a nanometer. This is achieved by scanning a tip over a surface and monitoring the motions of the tip in response to forces between the tip and surface. However, the AFM-generated image is not an exact replica of the real surface because tips are not infinitely thin and perfectly sharp. This can be confusing for students new to using the AFM, especially since the interaction between the AFM tip and the surface is imperceptible to the naked eye. It also underscores the risk of students perceiving the AFM as a black box, potentially impeding critical thinking about its fundamental principles and processes, which may lead to misinterpretation of AFM data. To address this learning gap and provide students with a more thorough understanding of AFM working principles, measurement inaccuracies, and the origins of image artifacts, we created and implemented an educational simulation. Students can use this simulation to explore diverse tip geometries on various surface topologies and observe the resulting images generated by the AFM. We have created activities and assessments that guide students to use the simulation to grasp key concepts related to tip-surface interaction and measurement accuracy. This module has now been released in both the undergraduate-level and graduate-level micro/nano-laboratory course (“Micro/Nano Engineering Laboratory”) at the Massachusetts Institute of Technology (MIT). We developed pre- and post-assessments to compare cognitive outcomes and learning experiences between simulation-based learning and traditional paper-based learning. Our user test with 36 students showed a strong preference for the simulation format over the paper format for learning about AFM image artifacts, with students valuing the simulation’s interactive nature.

Keywords: atomic force microscopy, image artifacts, educational simulation

1 Introduction

Nanoengineering brings together principles from physics, chemistry, biology, and engineering to design and manipulate structures and devices with dimensions on the nanometer scale. As nanotechnology progresses, there is an increasing necessity to educate a workforce capable of effectively utilizing these advancing technologies, with the introduction to nanoengineering ideally starting as early as middle school [1–3]. Nevertheless, there are numerous educational challenges, notably the stark contrast between our intuitive understanding of physical laws, which were developed at the macroscale, and the fundamentally different physics at work in the nanoscale [4]. Another challenge arises from the interdisciplinary nature of nanoengineering, potentially causing secondary educators to view it as a new science rather than recognizing it as a synthesis of various scientific and engineering topics [2]. Further, nanoengineering education is limited by the fact that expensive and sophisticated equipment, such as the Atomic Force Microscope (AFM) and the Scanning Electron Microscope (SEM), are needed to visualize materials at the nanoscale. This limitation may restrict hands-on learning opportunities and necessitate careful planning to effectively educate a large number of students [5]. To address these challenges, we advocate for the development of cost-effective nanoengineering and nanoimaging interactive educational systems. This approach enhances the overall educational experience, better preparing students to contribute to the progress and applications of nanoengineering across diverse fields.

With that objective in mind, our focus was directed towards enhancing the instruction of the AFM. AFM is an indispensable tool for researchers and engineers in nanotechnology, offering exceptional resolution in material visualization through the interaction of a tip with the surface material [6–8]. Nonetheless, the images generated by the AFM may not accurately represent the material surface due to the existence of image artifacts. These artifacts could stem from various sources, including tip-surface convolution effects, tip contamination, or tip breakage. This aspect is often not readily apparent to new AFM users, as the interaction between the AFM tip and the material surface is invisible to the naked eye. Consequently, students may accept the resulting image without critically examining it, potentially leading to misinterpretation of the data.

To promote greater critical thinking and demonstrate the basic working principles of the AFM along with potential measurement inaccuracies, we developed an educational simulation [*]. This simulation enables students to choose different tip geometries and surface profiles, enabling them to visualize the interactions between the AFM tip and the surface and observe the resulting AFM image. This encourages a more in-depth exploration of AFM working principles compared to a traditional paper format. Additionally, we developed supplementary teaching materials aimed at fostering exploration and identifying various scenarios that may lead to image artifacts. This exploratory approach aims to equip students with the skills to discern genuine features from artifacts in AFM images. Our user study of 36 students revealed a strong preference for the simulation method, with students appreciating its interactive nature. For affective learning gains, our study did not find any statistically significant differences between the simulation and paper format groups. However, the simulation cohort exhibited either comparable or superior performance in terms of average affective learning gains compared to the paper cohort. In the cognitive assessment, the paper cohort demonstrated greater gains than the simulation cohort, although this difference was not statistically significant.

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[*] The source code of our simulation is available at `https://github.com/leapgroupmit/LEAPGroup-MicroNano-AFM-ImageArtifacts`

2 Background

AFM image artifacts are unintended distortions, anomalies, or features present in AFM images that do not accurately represent the true topography of the scanned sample [9, 10]. These artifacts can arise from various sources and factors inherent to the AFM imaging process. The predominant source of artifacts stems from tip-surface convolution, wherein the shape of the AFM tip becomes convoluted with the surface features being scanned [9, 10]. This is illustrated in Fig. 1 where the AFM surface profile measurement (red line) differs greatly from the true surface profile (blue surface) due to the convolution between the tip (black shape) and the surface. Additional image artifacts can arise from tip failure modes, including tip contamination, where unintended foreign materials adhere to the tip [10, 11], sheared tips [12], or tips with multiple peaks, which can occur when a tip breaks [13]. Furthermore, there are two main modes of AFM operation. One is contact mode in which the AFM tip scans over a surface, and the surface profile is reconstructed by observing the motions of the tip in response to forces between the tip and surface. The other is tapping (or dynamic) mode in which the AFM tip is lowered to the surface, raised again, and moved across a certain distance before being lowered again. In this way, the tip only interacts with the surface at various intervals [14]. As these tip-surface interactions happen at the micro to nano-scale, they are invisible to the naked eye, making it challenging to comprehend the source of these image artifacts. Leveraging computer simulations serves as a valuable approach to illuminate these imperceptible interactions, aiding in the enhanced understanding of the sources of image artifacts.

Using simulations in the classroom is a useful tool to enhance learning, particularly when pre-

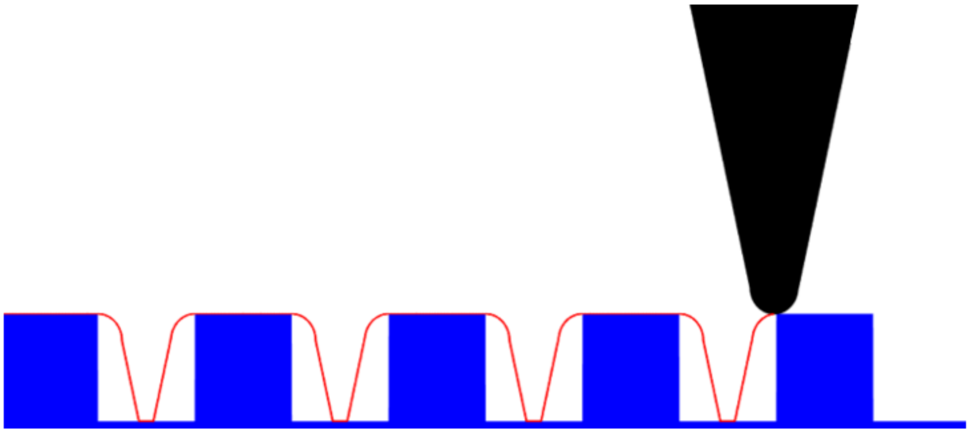

Figure 1: Tip-surface convolution image artifact. The square surface profile is shown in blue. The AFM tip is represented in black. The red line is the surface profile measurement by the AFM as the tip is scanned across the surface. Note that in the AFM surface measurement, the sidewalls of the square surface profile are wider and no longer vertical due to convolution with the tip shape.

sented with guided instruction [15–19]. Computer simulations are especially beneficial for visualizing phenomena that are inherently invisible [16]. Computer simulations have been used to teach such diverse scientific topics such as physics [20], chemistry [21, 22], the photoelectric effect [23], photonics [24], gas properties [25], mechanics of materials [26], and molecular biology [27, 28].

Several computer simulations have been created to teach about AFM operational principles. One such simulator is *VEDA* (Virtual Environment for Dynamic AFM), which focuses on tip and beam dynamics and surface interactions during dynamic AFM operation in various environments using precise mathematical models. In *VEDA*, a user can adjust various AFM operation settings, such as tip radius, tip hardness, cantilever stiffness, and resonance frequency and see their effects on the tip and surface interaction [29, 30]. J. Griffith has also created educational simulation tools, available online, to teach various working principles of AFM. For instance, *AFM Probe Simulator* enables users to observe AFM surface measurements based on different surfaces and probe tips that they can select. The user can control the animation of the tip's contact mode, observing its scanning process across the surface. Additionally, the *AFM Model* simulation allows users to adjust the feedback gain, scan speed, set reference, and sample height to show how the AFM measures the surface and generates images [31]. Heying et al. have also developed a virtual AFM simulator, which utilized a physics engine and a collision library to replicate the contact mode operation of an AFM. Users can manipulate AFM operation parameters, including scan rate, deflection setpoint, and PID gains, to observe their impact on a line scan between the tip and the surface, featuring a cylindrical log in the middle [32]. *BioAFMviewer* is a standalone software that transforms molecular structures into AFM-like graphics through simulated scanning with variable spatial resolution and tip-shape geometry [33].

In summary, existing AFM simulations typically focus on tip-shape convolution effects, overlooking other crucial image artifacts associated with contaminated tips, sheared tips, or tips with multiple peaks. Apart from J. Griffith's simulations, these simulations do not provide a visualization of the tip and surface interaction, providing only the final surface scan result. Moreover, the effectiveness of these simulations in teaching AFM principles has not been thoroughly examined. Therefore, our work seeks to fill this gap by creating a simulation that allows users to explore various tip and surface geometries, including different broken tips, and visualize how the surface measurement is generated. Thus, the simulation effectively illustrates the diverse artifacts that may appear in AFM images. Additionally, we aim to assess the effectiveness of our simulation in teaching AFM image artifacts through a user study.

3 Systems Design

Through multiple iterations of informal user testing, we developed and enhanced the AFM image artifacts simulation along with its accompanying educational materials. In this section, we elaborate on the design of the simulation and learning modules.

3.1 Simulation

Our AFM image artifacts MATLAB® application (app) can be installed either through MATLAB® or as a standalone program on a Windows computer. The user can choose from a selection of options in the AFM image artifacts app, as shown in Fig. 2. The options include the following, with each number corresponding to the respective numbers in Fig. 2:

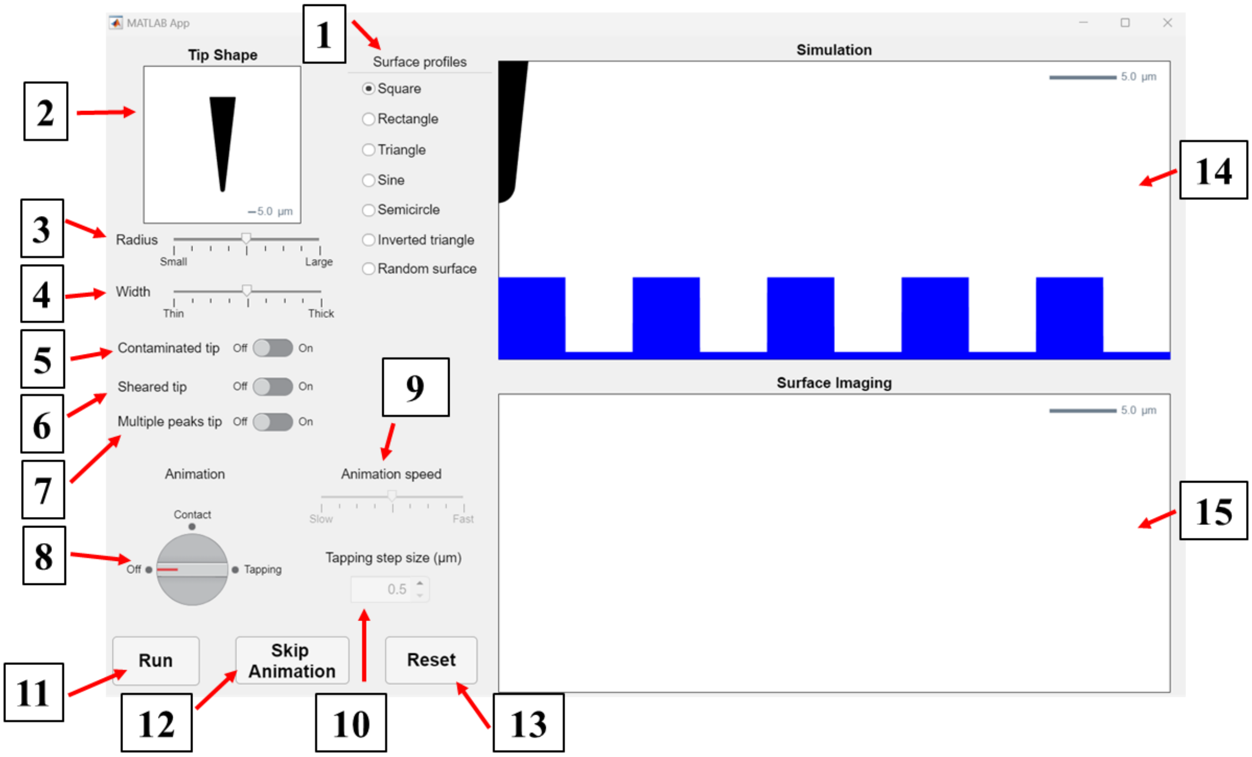

Figure 2: MATLAB® simulation application created to teach about AFM image artifacts. The app is comprised of the following components: **1** Surface Profile Selection, **2** Tip Shape Preview Window, **3** Tip Radius Slider, **4** Tip Width Slider, **5** Contaminated Tip Toggle, **6** Sheared Tip Toggle, **7** Multiple Peaks Tip Toggle, **8** Animation Knob, **9** Animation Speed Slider, **10** Tapping Step Size Spinner, **11** Run Button, **12** Skip Animation Button, **13** Reset Button, **14** Simulation Window, and **15** Surface Imaging Window.

1. Surface Profile Selection. The user can choose between various two-dimensional (2D) surface geometries of *Square*, *Rectangle*, *Triangle*, *Sine*, *Semicircle*, *Inverted Triangle*, and *Random Surface*. Each surface, with the exception of the *Random Surface*, is a repeating pattern of each surface profile option and is shown in blue in the Simulation Window of the app. As illustrated in Fig. 2, the selected surface profile is *Square*, which is shown as a repetitive pattern of square columns on a flat surface in the Simulation Window. The *Random Surface* consists of various 2D surface profiles combined together without a discernible pattern.

2. Tip Shape Preview Window. This window displays a preview of the tip, generated based

on the user's selections.

3. Tip Radius Slider. The user can modify the tip radius using the slider, ranging from *Small* (resulting in a pointed tip) to *Large* (resulting in a large semicircular tip).
4. Tip Width Slider. The user can modify the tip width using the slider, ranging from *Thin* (where the top of the tip matches the diameter of the selected tip radius) to *Thick* (where the top of the tip is much wider than the diameter of the chosen tip radius). The tip shown in Fig. 2 has a *Medium* radius and *Medium* width.
5. Contaminated Tip Toggle. Enabling this option will result in a contaminated tip, altering the tip profile to be more irregular, mimicking real-life scenarios where sample residues or dust could adhere to and contaminate the tip [11].
6. Sheared Tip Toggle. Enabling this option will result in a broken tip, where the end of the tip has been sheared off at an angle.
7. Multiple Peaks Tip Toggle. Enabling this option will result in a broken tip with multiple peaks at the the end.
8. Animation Knob. The user can adjust the type of animation and type of imaging shown in the Simulation and Surface Imaging Windows. The options include *Off*, *Contact*, and *Tapping*. No animation is shown for the *Off* option. The *Contact* animation demonstrates the AFM contact operation mode, and the *Tapping* animation demonstrates the AFM tapping operation mode.
9. Animation Speed Slider. If either the *Contact* or *Tapping* animations are chosen, this slider is enabled and the user can adjust the speed of the animation from *Slow* to *Fast*.
10. Tapping Step Size Spinner. If the *Tapping* animation is selected, then the user can adjust tapping step size, representing the interval distance between taps of the AFM tip with the surface.
11. Run Button. Once pressed, the resulting surface image produced by the user's selections is calculated according to the algorithm developed by J.S. Villarrubia [34] (see Appendix A for more details) and the tip animation, if any, is shown.
12. Skip Animation Button. Once pressed, this button allows the user to skip to the end of the animation before it finishes.
13. Reset Button. Once pressed, the app will revert back to its default settings.
14. Simulation Window. The animation is shown in this window.
15. Surface Imaging Window. The AFM surface measurement is shown as a red line in this window once the Run button is pressed.

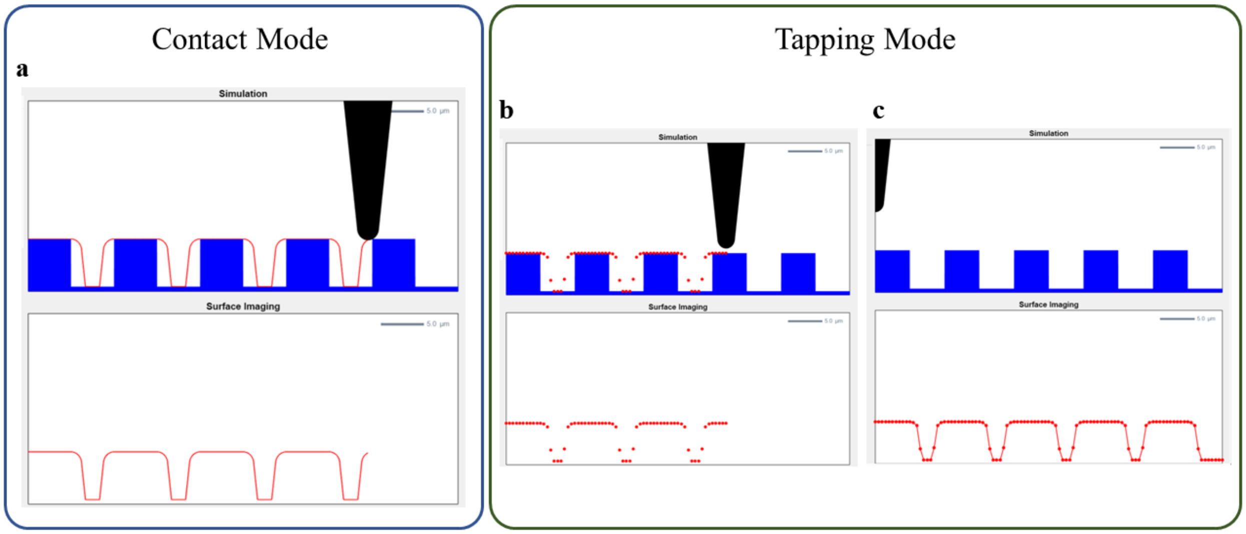

Figure 3: Screenshots of the simulation demonstrating contact and tapping modes of operation for the AFM. **a** Simulation screenshot of contact mode, showing the red line of the surface measurement being drawn as the tip scans the surface. **b** Simulation screenshot of the tapping mode before the animation is completed, showing the red dots, which represent the measurement points as the tip interacts with the surface. **c** Simulation screenshot of the tapping mode after the animation is completed, showing the resulting surface measurement as the red line connecting the measurement points.

Only one tip failure mode can be active at a time. For instance, if the sheared tip toggle is switched on, the contaminated tip and multiple peaks tip toggles would be disabled and appear grayed out.

If Contact mode is chosen, the animation shows the tip moving across the surface, and the AFM surface measurement is shown as a red line in the Simulation and Surface Imaging windows as the tip is scanning the surface profile (see Fig. 3a). If Tapping mode is chosen, the animation will show the measurement points of the tip as it taps across the surface as red dots in both the Simulation and Surface Imaging windows (see Fig. 3b). Once the tapping animation is completed, a red line connecting the measurement points will appear in the Surface Imaging window demonstrating the surface measurement (see Fig. 3c).

This app enables learners to investigate various tip geometries and observe their impact on the resulting surface measurement produced by the AFM (see Fig. 4). Additionally, the app displays both the true surface profile and the resulting AFM surface measurement, allowing learners to make a direct comparison. By rendering this typically invisible process visible, learners can enhance their understanding of the origins of AFM image artifacts.

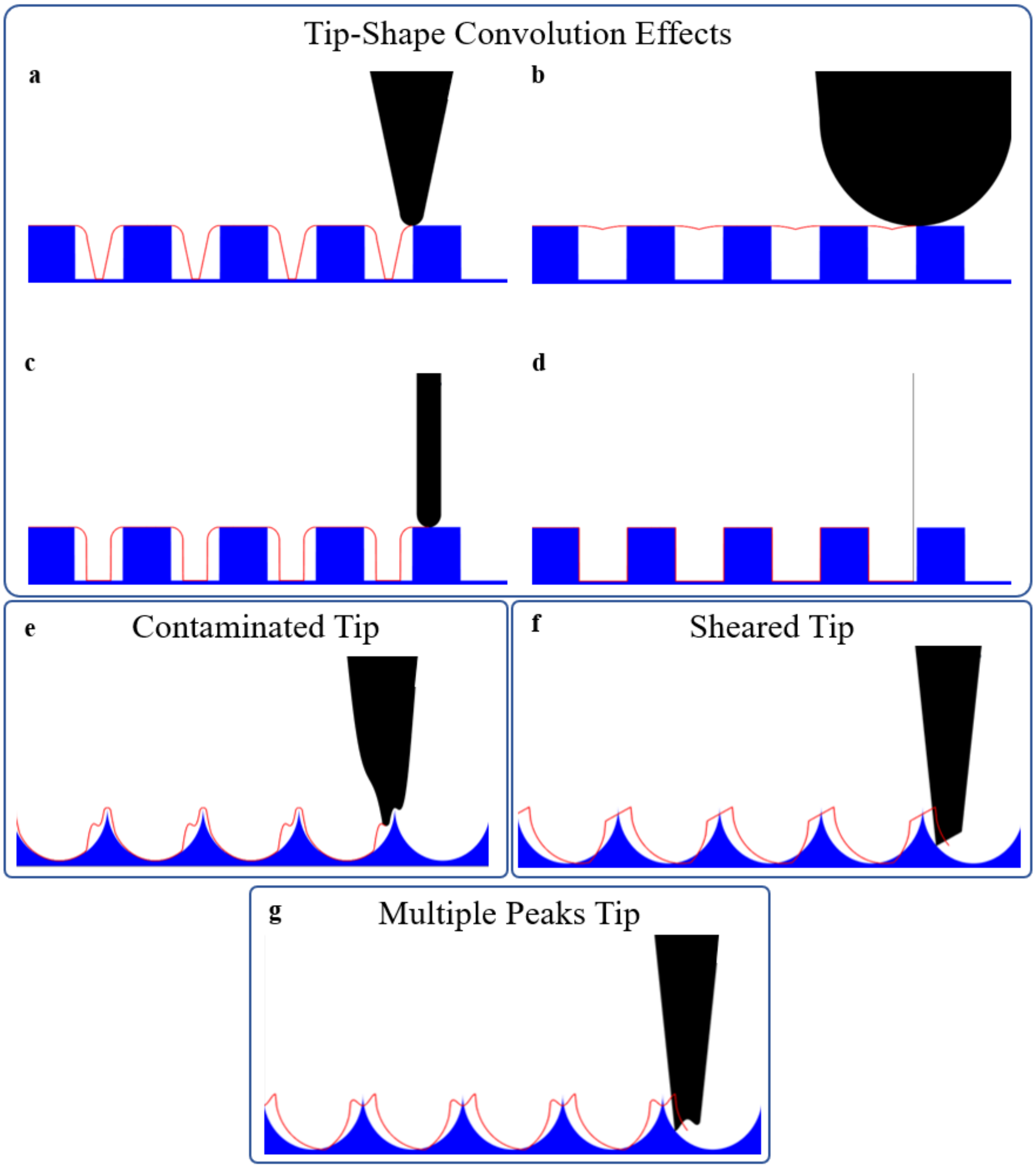

Figure 4: Screenshots of the app's Simulation window illustrating the effect that diverse tip geometries have on the surface measurement generated by the AFM. The learning module concentrated on frequently encountered AFM image artifacts, including **a** - **d** tip-surface convolution effects and the tip failure modes of **e** contaminated tip, **f** sheared tip, and **g** a tip with multiple peaks. **a** *Medium* radius and *Thick* width tip **b** *Large* radius and *Thick* width tip **c** *Medium* radius and *Thin* width tip **d** *Small* radius and *Thin* width tip. The tips in **a** - **d** image the *Square* surface profile. **e** Contaminated tip toggle enabled with a *Medium Small* radius and *Medium Thick* width. **f** Sheared tip toggle enabled. **g** Multiple peaks tip toggle enabled. The tips in **e** - **g** image the *Semicircle* surface profile. Note that only the impossibly sharp and thin tip depicted in **d** accurately images the surface profile.

3.2 Learning Module

In the learning module, the students are prompted to select a specific tip shape and surface profile. Then, they need to predict what the resulting AFM surface measurement would be before observing the actual result. This "predict first" methodology is found to improve learner retention [35] and designed to enhance critical thinking skills by prompting them to evaluate (or reevaluate and reconcile) their assumptions [36]. At the end of each teaching section, there is a concept question to evaluate the learners' understanding. The learning materials concentrated on the most common of AFM image artifacts, namely, tip-surface convolution effects (Fig. 4a-d), contaminated tips (Fig. 4e), sheared tips (Fig. 4f), and tips with multiple peaks (Fig. 4g). Because the app only shows 2D surface profiles, a section of the learning module guides learners on how the AFM images three-dimensional (3D) surfaces. Employing only text and figures, this section of the learning module illustrates what these tip failure modes look like in 3D, utilizing real AFM images.

4 User Testing

To evaluate the effectiveness of simulation-based learning compared to a traditional paper-based learning in terms of learner preferences, learner experiences, and cognitive outcomes, we developed pre- and post-assessments (also called pre-/post- labs), learning materials, and a learner preferences survey. We designed this study so that it can be completed within one hour in a lab session of a micro/nano-laboratory course that is offered at MIT.

4.1 Study Participants

The study was conducted in a micro/nano-laboratory course offered in the Spring and Fall semesters of 2023. This lab-based course introduces students to various topics in nanoengineering. These include microfludics, microelectromechanical systems, nanomaterials, and nanoimaging tools such as the AFM and SEM. The Spring semester version is offered to undergraduate students, and the Fall semester version is offered primarily to graduate students, although undergraduates can also take the course in the Fall semester. The material taught between the undergraduate and graduate versions of the course are similar, with the graduate students having more in-depth lectures and an extra project assignment. Because this is an introductory course on nanoengineering, a wide variety of students take this course. Although the majority of students enrolled in the course major in mechanical engineering, there is a diverse variety of majors represented, including aerospace engineering, electrical engineering, biological engineering, media arts and sciences, health sciences and technology, and management. Most undergraduate students taking this class have little to no experience in nanoengineering and nanoimaging, whereas some of the graduate students are starting to pursue research in small scale engineering and science. In the Spring semester, 13 undergraduate students completed this study. In the Fall semester, there were 23 participants: 22 graduate students and one undergraduate student. Due to time constraints during the Spring and Fall semesters, our study was carried out after the students had received instruction on the AFM in class and had practical exposure to the actual equipment.

4.2 Study Procedure

The flow chart of the user test is shown in Fig. 5. All the students completed the same pre-lab which consists of affective and cognitive assessments. The students were given access to the pre-lab several days prior to the lab session and were instructed to complete it beforehand. Thus, the students could take as much time as they wanted to complete the pre-lab. The pre-lab was the only step completed outside of the lab session. All other steps in the flow chart were conducted during the lab session.

The affective assessment used in the pre-lab is a survey comprising of 19 questions, which were adapted from the Motivated Strategies for Learning Questionnaire (MSLQ) [37, 38], to measure attitudes associated with learning. In this survey, the learner is asked to rate statements on a 7-point Likert scale (1 - “not at all true of me” to 7 - “very true of me”). The students rated their attitudes toward intrinsic goal orientation, which is associated with a student’s perception that they should participate in the learning task because it is challenging, arouses their curiosity, and for complete understanding of the material. Further, the students rated their motivation to reengage with the material and their fear of making mistakes. Finally, the survey also asked the students to rate several self-efficacy constructs, where they are asked to judge their ability to learn the material, apply the material they have learned, and how well they believe they will perform in the

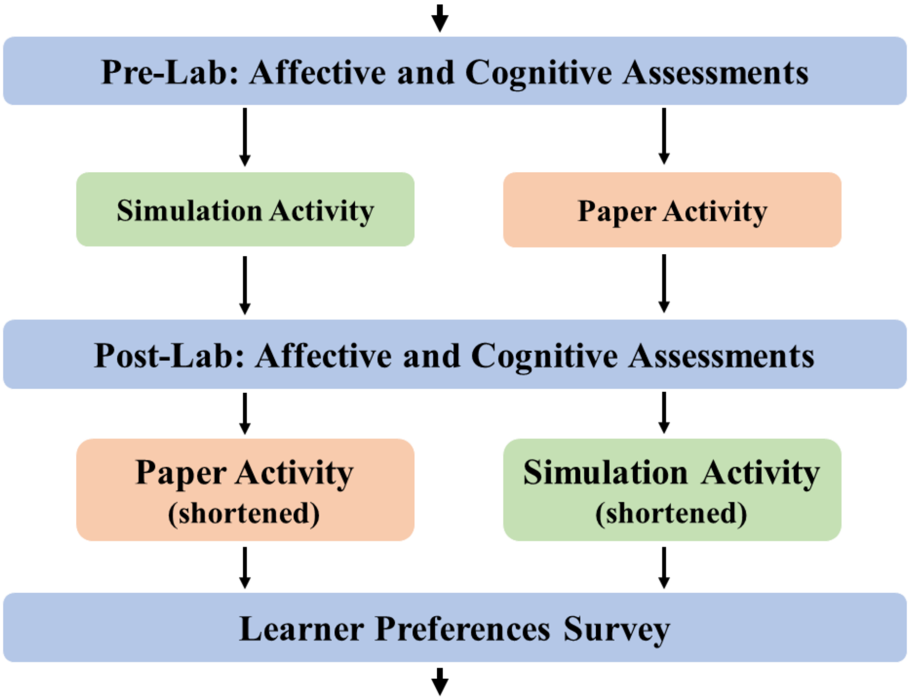

Figure 5: User testing flow chart.

learning activity. The full list of questions in the affective assessment is provided in Appendix B. The cognitive assessment consists of five multiple-choice questions focusing on technical aspects of AFM imaging and identifying sources of common image artifacts.

In the lab session, once it was confirmed that each student had completed the pre-lab, they were randomly assigned to either the simulation cohort or the traditional paper (control) cohort. Students in the paper cohort did not have access to the simulation and were instead provided with image(s) generated by the simulation, illustrating the concept being taught. The biggest difference between the two activities was that the paper version did not allow the students the ability to explore further with different tip geometries or surface profiles. In the Spring 2023 semester, six students were in the paper group while seven students were in the simulation group. In the Fall 2023 semester, 12 students were in the paper group while 11 students were in the simulation group. Irrespective of the format, students worked independently on the learning activity, with an instructor available to answer questions as they circulated around the room. At the end of the learning activity, learners had the opportunity to see and review the solutions.

Following the learning activity, all students took the post-lab assessment. The affective assessment in the post-lab used the same 19 questions of the affective assessment in the pre-lab. The students also answered five new multiple-choice technical questions of AFM imaging for the cognitive assessment portion of the post-lab. The post-lab cognitive questions were designed to have the same level of difficulty as the pre-lab cognitive questions. After completing the post-lab, the students completed a shortened version of the other format. Put differently, if a student did the simulation activity after the pre-lab, they completed a shortened version of the paper activity after the post-lab.

After finishing this shortened activity, students completed a survey gauging their learning preferences. They were prompted to rank statements on a 7-point Likert scale (1 - “not at all true of me” to 7 - “very true of me”) regarding the perceived usefulness of the material, their enjoyment using the simulation, and their preference for using the simulation over traditional text and graphics (see Appendix C and Fig. 6 for the full statements). The students could also provide open-ended responses to specific optional questions about the learning activity, including whether the simulation enhanced or hindered their learning, and any additional feedback they wished to share (refer to Appendix C and Fig. 7 for the complete statements).

5 Analysis and Results

We analyzed the learner preferences and compared affective and cognitive learning gains between the simulation and paper format groups. The simulation and paper cohorts each consisted of 18 students, when the data is combined across the Spring and Fall semesters.

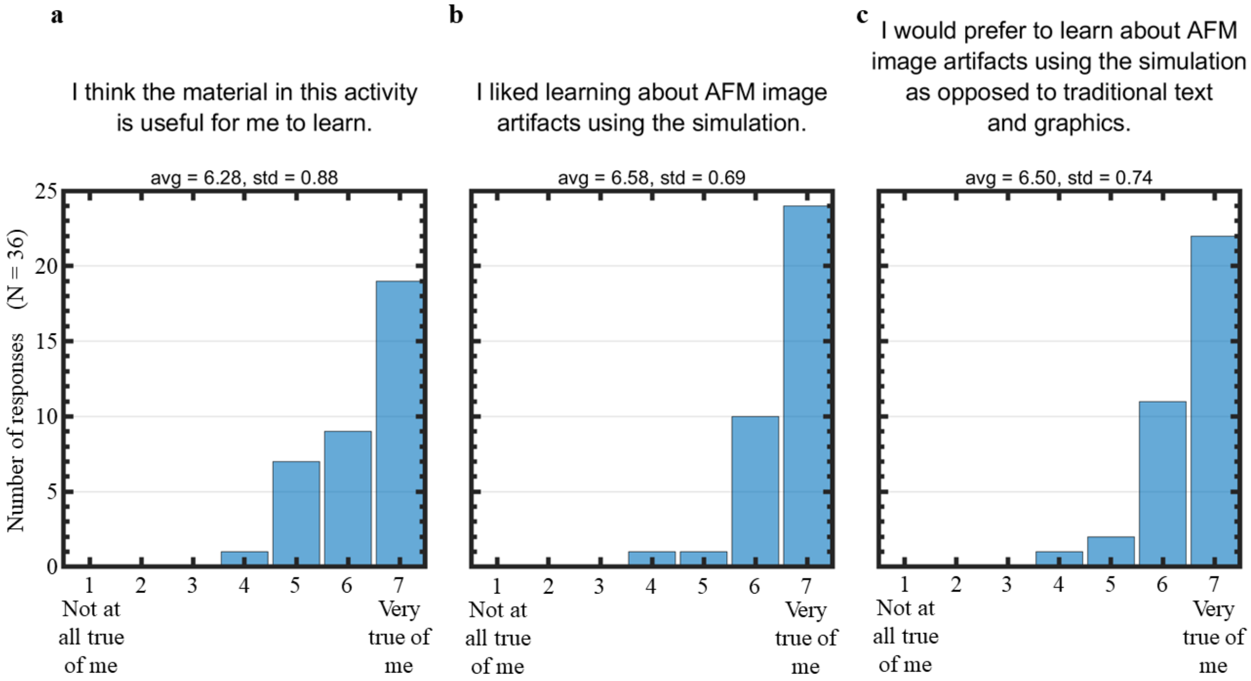

Figure 6: Learner preferences. The statements that learners are prompted to rank in the learner preference survey are displayed above each histogram. Learners from both the simulation and paper cohorts strongly favored the simulation learning format over the paper learning format.

5.1 Learner Preferences

The results for the learner preferences survey are shown in Fig. 6. To examine if there were any potential bias due to the order in which students completed the formats, we first conducted normality checks using the Shapiro-Wilk test ($\alpha_{SW} = 0.05$) and Q-Q plots. Because none of the samples were normally distributed ($p_{SW} < 0.05$), we used the non-parametric Mann-Whitney U test ($\alpha_{MWU} = 0.05$) to compare the simulation cohort with the paper cohort for each preference statement. We found that there was no statistically significant difference between the simulation and paper cohorts. Thus, irrespective of whether learners tried the simulation learning format before or after the paper format, they consistently favored the simulation. Notably, even though the paper cohort completed only a shortened version of the simulation activity, they still expressed a preference for the simulation format.

Two of the authors collaboratively classified the open-ended responses from the learner preference survey (see Appendix D) into positive, negative, or neutral sentiment categories. Comments categorized as providing constructive feedback, such as offering suggestions for improvement, were classified as neutral sentiment. This classification was made because these comments did not exhibit strongly positive or negative opinions but rather presented a balanced evaluation of the learning activity. The results are shown in Fig. 7 for each question. Figure 7a shows predominantly positive comments, with few negative remarks and no neutral observations. Figure 7b

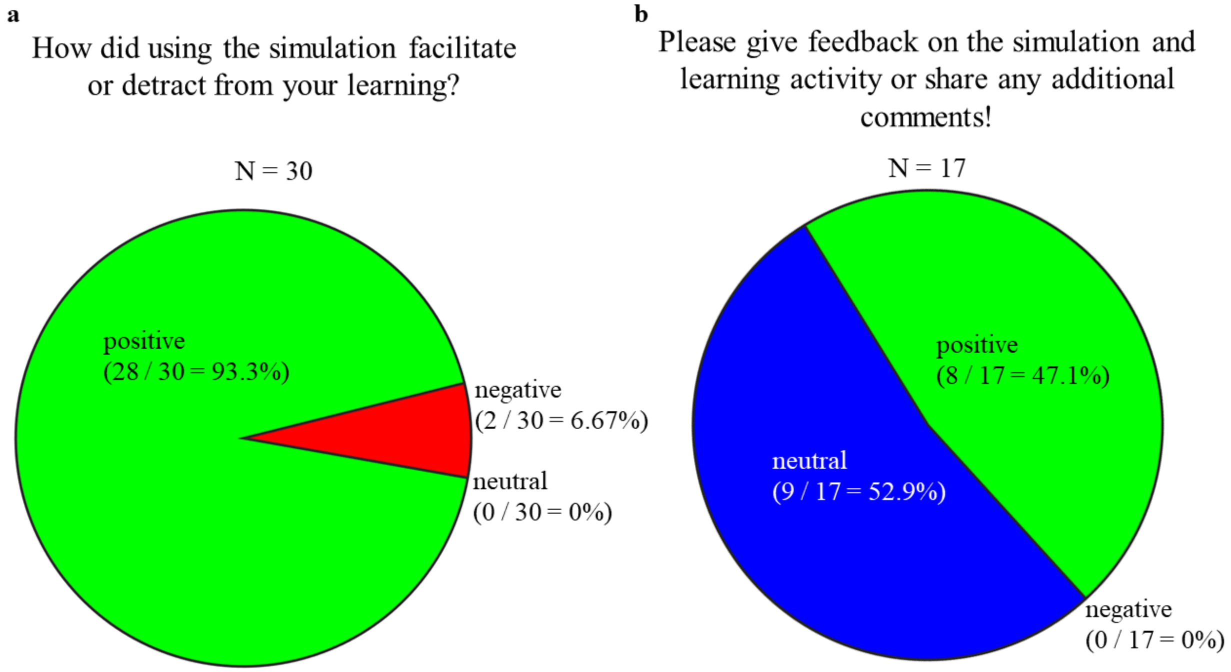

Figure 7: Sentiment analysis pie charts. Most statements for each question are either positive or neutral, with few negative responses.

depicts a nearly equal distribution between positive and neutral responses, with no negative comments provided.

5.2 Learning Gains

When assessing the affective and cognitive outcomes between the simulation and paper formats, we chose to compare using the students' individual learning gains so that we account for the students' prior learning attitudes and knowledge. To calculate this gain, we used the normalized change c defined by J. D. Marx and K. Cummings [39], which is reproduced below for convenience.

$$c = \begin{cases} \frac{post - pre}{100 - pre} & post > pre \\ \frac{post - pre}{pre} & post < pre \\ \text{drop} & post = pre = 100 \text{ or } 0 \\ 0 & post = pre \end{cases} \tag{1}$$

where *pre* and *post* refer to the pre-score and post-score out of 100%, respectively. c is normalized so that the gains or losses are compared with their maximum possible gain or loss. Additionally, c is excluded if the student achieved 0% for both the pre-score and post-score for each assessment, as there is no discernible improvement or decline when the student scores the minimum for both assessments. The same is true if the student scores 100% for both the pre-score and post-score. If the pre-score and post-score are equal, but not equal to 0% or 100%, then $c = 0$. There are no gains or losses in this case. From Eq. (1), we see that $-1 \leq c \leq 1$ [39]. In this work, we will also refer to c as the normalized learning gain.

With the exception of assessments related to fear of mistakes, the scoring of all assessments correlated higher scores with improvement. To standardize the correlation between higher scores and improvement for all assessments, we inverted the survey results to statements 2 and 14 in the MSLQ (see Appendix B) in the fear of mistakes assessment, such that a 7 is now a 1, a 6 is now a 2, and so on. (Statement 19 in the MSLQ already aligned with this scoring.)

By applying the calculation detailed in Eq. (1) to each learner's pre- and post-assessment responses, we examined the distribution of the normalized learning gain for both the simulation and paper cohorts. The percentages of the total survey responses that are in each category in Eq. (1) are shown in Appendix E. Across all of the assessments, the average number of responses that were dropped were 17.9% and 5.6% for the simulation and paper cohorts, respectively. Given the non-normal distribution of all c distributions for each assessment (validated through the Shapiro-Wilk test with $p_{SW} < 0.05$ and Q-Q plots), the Mann-Whitney U test ($\alpha_{MWU} = 0.05$) was used to compare the simulation and paper cohorts for each assessment. The results are shown in Table 1. Despite the absence of statistically significant differences between the two format groups in any of the assessments, it is noteworthy that, when comparing the averages and rank sum means, the simulation format consistently exhibits either comparable or superior normalized learning gains in all affective assessments compared to the paper format. Conversely, in the cognitive assessment, the paper format demonstrates larger normalized learning gains than the simulation format, albeit without statistical significance.

6 Discussion

6.1 Learner Preferences

The students strongly favored the simulation learning format over the paper learning format, as illustrated in Fig. 6c, where nearly all learners indicated that they would prefer learning using the simulation format over the paper format. Importantly, there is no statistically significant difference between the simulation and paper format groups regarding learner preferences statements. Thus, regardless of which format the student completed first (and note that the students that completed the paper format first only did a shortened version of the simulation activity after the post-lab), learners of both cohorts preferred the simulation format. This preference is further supported by the sentiment classification results shown in Fig. 7a, indicating that 93.3% of the learner responses were positive, while only 6.67% were negative to whether the simulation facili-

	Simulation			Paper				
Assessment	avg	std	$\bar{R}$	avg	std	$\bar{R}$	U-stat	p
intrinsic goal orientation	0.26	0.53	44.10	0.25	0.40	45.74	944	0.622
motivation to re-engage	0.28	0.44	49.71	0.27	0.31	50.28	1210	0.541
fear of mistakes	0.24	0.54	46.05	0.10	0.40	38.41	700	0.071
self-efficacy: learning	0.28	0.51	45.65	0.23	0.39	45.38	988.5	0.482
self-efficacy: application	0.41	0.44	68.01	0.33	0.38	61.59	1826.5	0.164
self-efficacy: performance	0.24	0.49	50.28	0.22	0.31	51.63	1235	0.596
cognitive	0.36	0.42	16.61	0.46	0.57	20.39	128	0.865

Table 1: Statistics for the normalized learning gains for affective and cognitive assessments. Reported in the table are the average, standard deviation, and rank sum mean $\bar{R}$ of the normalized learning gains for each cohort, the U-stat, and the p value. There are not statistically significant differences between the simulation and paper cohorts for all assessments.

tated or detracted from learning.

Notably, a significant majority of learners found the material useful for learning regardless of format, as illustrated in Fig. 6a. This suggests that while the content itself is perceived as valuable, the mode of instruction does impact preferences, with a distinct preference toward the simulation format in this case.

This may be due to the fact that the simulation format is more interactive than the paper format. Observations during the lab sessions indicated that students starting with the simulation format took longer to complete the learning activity, possibly due to their interest in experimenting with additional settings beyond those specified in the teaching activity. This interactivity of the simulation was commented on frequently in the open-ended responses, examples include:

- *It was cool to be able to play around with different tips and directly see the impact of different flaws on the image it produced.*
- *Really liked the simulation. Very interactive and really helps us understand all the common possible problems in AFM without the need to have very expensive equipment and/or samples.*
- *The simulation is great. Being able to change the parameters on the simulation to test different scenarios is very useful, especially after reviewing the material and having more questions arise.*

6.2 Learning Gains

In all assessments, both the paper and simulation formats demonstrated a positive average normalized learning gain. Consequently, both formats proved effective in enhancing students' performance in both affective and cognitive assessments. Concerning intrinsic goal orientation, motivation to reengage, self-efficacy for learning, and self-efficacy for performance, the averages of normalized learning gains and the rank sum mean comparison of each format are comparable between the simulation and paper format groups. Although not statistically significant, this suggests that, in these categories, both simulation and paper formats aided students to a similar extent.

For the self-efficacy application assessment, the average normalized gain was higher for the simulation than the paper format (averages of 0.41 vs 0.33). These statements refer to an individual's confidence in understanding and addressing various aspects related to AFM image artifacts. This could be due to the fact that the simulation presents an animated depiction of AFM operation, unlike the static images in the paper format. Hence, students can directly observe the real-time functioning of the AFM instead of relying on imagination, aligning with literature emphasizing the effectiveness of animations in teaching dynamic changes [40]. Numerous students noted that the simulation facilitated them in either "seeing" (as mentioned in seven statements) or "visualizing" (as mentioned in five statements) the scanning process of the AFM.

In the fear of mistakes assessment, the average normalized gain in the simulation format greatly surpassed that in the paper format (averages of 0.24 vs 0.10). Further, the majority of the paper format normalized gains are near 0, whereas the simulation format showed a larger spread of positive gains (see Fig. 10c in Appendix F). This difference is likely attributable to the low-risk interactive environment of the simulation format, which enables exploration without adverse consequences [41, 42]. One student stated, "[I]t was helpful to see the outcome generated by the tip as it went. It made it easier to try out things rather than intuit outcomes."

The students rated themselves similarly on how well they will perform on the activity (averages of 0.24 vs 0.22), but the paper format group performed better on the cognitive assessment than the simulation group (averages of 0.36 vs 0.46). This suggests that students in the paper group showed greater comprehension of the material compared to those who used the simulation format, although this is not statistically significant. This could be attributed to the novelty and openness of the simulation format where the information transfer is less straightforward than in the paper format [17, 18]. Moreover, the pre- and post-tests consisted of only five multiple-choice questions each, making a single additional correct or incorrect answer significantly impactful on the results. Including additional questions in the pre- and post-cognitive tests would offer a more detailed assessment of the effectiveness of each format in educating students about AFM image artifacts. Also, several students mentioned how it was hard to make the transition from 2D profiles to 3D images and stated that a simulation of 3D profiles would be helpful (as mentioned in six statements).

7 Conclusion and Future Work

We created an educational simulation which demonstrates the tip-surface interaction of AFM imaging in order to provide students with a more complete understanding of AFM working principles. This simulation is cost-effective and easily scalable, enabling multiple learners to utilize their individual copies simultaneously. This simulation approach also allowed students a more open-ended learning experience than traditional paper format. The results of our user study, involving 36 students, demonstrated a clear preference for the simulation format over the paper format, which suggests the simulation's potential effectiveness in engaging students and fostering a deeper curiosity of nanotechnology. While not statistically significant, the simulation format exhibited either comparable or superior performance to the paper format in terms of affective normalized learning gains, whereas the paper format showed larger normalized gains than the simulation format in the cognitive assessment, though this is not statistically significant.

There are several ways to improve this study. First, our sample size is fairly small, consisting of only 36 students with various levels of exposure to nanoimaging. A more accurate measurement of the normalized learning gains between the two formats could be achieved by conducting a larger study with learners that have little to no prior exposure to nanoimaging. Moreover, the cognitive questionnaire for both the pre-lab and post-lab could be expanded to include more than five questions each. Increasing the number of questions will mitigate the impact of a single correct or incorrect response in the cognitive learning gain measurement, ensuring a more nuanced and accurate evaluation of cognitive outcomes. Further, the simulation could be improved such that it included an extension of how 3D profiles are measured to better mimic the actual operation of the AFM. Implementing these suggested improvements would enhance our understanding of the effectiveness of the simulation format in teaching AFM image artifacts.

In summary, our results underscore the promise of the AFM image artifacts educational simulation as a highly interactive and easily scalable teaching tool. This approach not only addresses financial and logistical barriers in nanoengineering education but also equips students with essential technical skills for proficient AFM use, fostering heightened curiosity and interest in nanoimaging.

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Appendices

Appendix A AFM Visualization Algorithm

The surface profile and tip shape are discretized (with the same step size) with a large number of points. When the bottom midpoint of the tip is at initial position (x_t, y_t) above the surface, we find the minimum vertical distance, d, between the tip shape and the surface profile. In essence, we are finding the smallest distance between any point on the tip and the surface profile, thus identifying the point of first contact that the tip would make with the surface. The resulting surface image coordinate (x_i, y_i) would be the coordinate of the bottom midpoint of the tip minus this minimum distance [34]. In other words,

$$x_i = x_t - d \tag{2}$$

$$y_i = y_t - d \tag{3}$$

This sequence is performed over the entire surface profile to find the resulting AFM surface image produced by tip the user selected of the surface profile.

Appendix B Motivated Strategies for Learning Questionnaire (MSLQ)

The numbers before each statement refer to its location in the questionnaire.

Intrinsic Goal Orientation

6. The most satisfying thing for me in this activity is trying to understand the content as thoroughly as possible.

12. In an activity like this, I prefer material that arouses my curiosity, even if it is difficult to learn.

15. In an activity like this, I prefer material that really challenges me so I can learn new things.

Motivation to Re-engage

1. I look forward to the next time I'll be able to engage with AFM imaging.

4. I see myself engaging with AFM imaging for a long time to come.

8. I will seek out opportunities to engage in AFM imaging outside of required MechE courses (e.g. electives, independent/club projects).

Fear of mistakes

2. I'm afraid of trying new things because of my fear of making mistakes. *

---

*survey responses were reversed to align with the other assessments

14. I fear that my own errors may impede my learning progress. *

19. I believe that making mistakes is a natural part of the learning process.

Self-efficacy - Learning

7. I’m certain I can understand the most challenging material presented in the AFM Image Artifacts activity.

9. I’m certain I can master the content being taught in this activity.

16. I’m confident I can understand the basic concepts taught in the AFM Image Artifacts activity.

Self-efficacy - Application

3. I’m confident I can explain why AFM image artifacts occur.

10. I’m certain I can recognize common sources of image artifacts created by the AFM.

13. I’m confident in my ability to determine whether an AFM image requires re-imaging with a new tip.

17. I’m confident I can explain what AFM image artifacts are.

Self-efficacy - Performance

5. I expect to do well in the AFM Image Artifacts activity.

11. I’m confident I can do an excellent job on the tasks of the AFM Image Artifacts activity.

18. Considering the difficulty of this activity and my skills, I think I will do well in the AFM Image Artifacts activity.

Appendix C Learner Preference Statements and Questions

Learner Preference Statements

- I think the material in this activity is useful for me to learn.
- I liked learning about AFM image artifacts using the simulation.
- I would prefer to learn about AFM image artifacts using the simulation as opposed to traditional text and graphics.

Learner Preference Optional Questions

- How did using the simulation facilitate or detract from your learning?
- Please give feedback on the simulation and learning activity or share any additional comments!

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*survey responses were reversed to align with the other assessments

Appendix D Learner Preference Open-Ended Responses

How did using the simulation facilitate or detract from your learning?

1. It helped visualize how the tip contacts the sample
2. It allowed me to visualize how AFM captures its images and understand its limitations
3. i could watch the tip moving over the surface as opposed to static graphics
4. It was cool to be able to play around with different tips and directly see the impact of different flaws on the image it produced.
5. It helped to be able to try out different tip sizes and various factors in a simulation to check my knowledge.
6. The simulation helped with my learning significantly.
7. It helped with imagining what a tip would look like with the defects
8. it showed me how the tip moves across the surface and how the shape of the tip appears in the scan as the profile gets traced out.
9. Being able to see what different tip shapes would change instantaneously taught me why some images look certain ways under an AFM.
10. It was useful to see how the type moved and contacted with the surface which made it easier to visualize why an AFM profile looks like it does
11. Interesting to play around with the different settings.
12. quite visible I like it
13. Really liked the simulation. Very interactive and really helps us understand all the common possible problems in AFM without the need to have very expensive equipment and/or samples.
14. It helped visualize corner/edge effects better by showing the tip geometry directly next to the surface profile.
15. I like how it visualizes the AFM process, making what I learn on paper be applied in a real practice way.
16. Made things more interactive
17. it was good to see the scanning process, but the given questions were too simple/i can imagine them without the simulation. I would need help with the more complicated/damaged tip cases. Those are the ones I cannot imagine as well when looking at two images side by side.

18. I thought it was very useful to test out my own hypotheses
19. The simulation was great. I think it was helpful to experiment with different settings in order to gain an intuition.
20. The simulation is facilitate my learning. I would also add the scale/ratio of the radius and the width compare to the scale of the measuring surface. So we can also understand that if we can to measure a certain sized feature what is the best range of tip size and width for the measurement.
21. The simulation is great. Being able to change the parameters on the simulation to test different scenarios is very useful, especially after reviewing the material and having more questions arise.
22. I think that since there was no real example that corresponded to the profiles in the simulation, it was hard to discern the optimal AFM tip/features for the scenarios in question.
23. Visually better to understands
24. It helps quickly understand where artifacts come from.
25. Facilitate
26. I liked the clear instruction, modification of dials/settings, and seeing how that changes the result. I also like the introduction of artifacts (broken tip, dirty tip, etc.) on top of dialing the AFM settings.
27. it was helpful to see the outcome generated by the tip as it went. It made it easier to try out things rather than intuit outcomes
28. Simulation help understand how different conditions of the tip will influence the imaging quality in a direct way
29. It facilitated it by showing how the tip would be moving across the surface and what the tip in the different scenarios actually looked like
30. The simulation for the 2D graphs was really good as a way to double check my understanding. I did not have an issue with the 2D graphs, but once we went to 3D, it was a bit harder for me to understand the exact defects that I was viewing. I feel like if the tool had a 3D view side by side to it, it would definitely enhance my learning, since in the real world, when we see AFM images, we do see them as 3D rather than just profiles.

Please give feedback on the simulation and learning activity or share any additional comments!

1. How would you image an inverted triangle? Is it possible?
2. it was hard for me to extrapolate the 1d scan graphs to the 2d scan pictures. If there was a way to simulate the tip in 3d that would be more intuitive

3. I liked the activity! It may be helpful to include more real images in the learning parts before the assessment. I felt that I understood how the linear profile should look but a harder time connecting that to how that would affect/look like as a flat image.
4. Would be helpful to have a version that allowed us to see the full image result, not just the 2D plot in the simulation.
5. Simulation is very cool! Straightforward to use and intuitive to set up.
6. Awesome simulation!
7. I guess i'm still unconfident in identifying the differences between contaminated,shear, and dull in actual images. I can recognize them in the given 2D profiles, but they all just look kind of blurry IRL. I can identify the double peak due to the shadow/doubling , though.
8. Great!
9. feedback over, also I think a sheared tip and a contaminated tip artifact can look very similar depending the resulting shape. Lookin gat the surface imaging in 2D with the red line it is hard to imagine it in a 3D plan structure (when the line is layered into the surface). One thing you could add for the simulation is to have the simulated "line" layered into a surface so we can see what it would look like in 3D. Or take a slice of the AFM 3D image and converted back into "line" to compare it to the simulation.
10. Liked the simulation very much. The only feature I would add is a top view of the artifacts. This could be either in the form of a drawing, like the section provided, or even having a couple of examples from the literature, like the ones shown in the previous google forms, would be nice. Just to familiarize with what an artifact in an image would look like, and being able to translate this faster in real time.
11. Thank you for making this, it helped me understand so much more!
12. It was more straight forward
13. I really like UI, I found it easy to use. I love the instructions and the order that you gave them. Maybe give another question where we can play with all the settings more free form?Thanks for sharing your work with us!!!
14. more examples can be given for the sheared tips
15. I think some of the wording (such as double images) for multiple peaks is a bit misleading; multiple peaks could mean 3 peaks, which means triple images right?
16. The user interface could be more asthetical
17. It would be useful if you could slow down the simulation further or pause it so you could look at how the tips are interacting with the corners of surfaces a bit better

Appendix E Normalized Learning Gains Statistics Plots

The percentages of the total survey responses that are in each category in Eq. (1) are shown below for the simulation, Fig 8, and for the paper, Fig. 9. In the legends, “drop 100” refers to the responses that were dropped because both the *pre* and *post* were equal to 100%. Likewise, “drop 0” in the legends refers to the responses that were dropped because both the *pre* and *post* were equal to 0%.

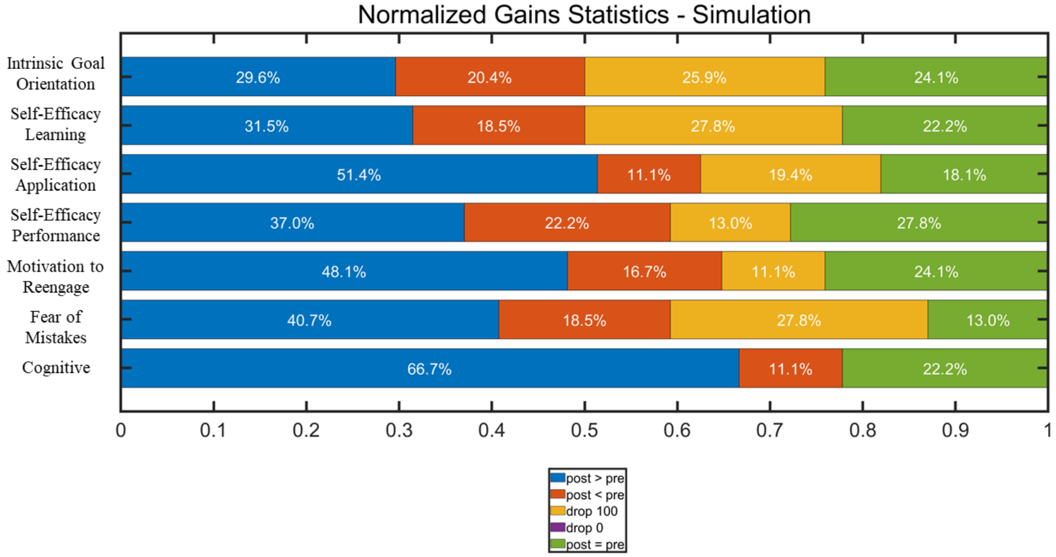

Figure 8: Normalized learning gains statistics: simulation.

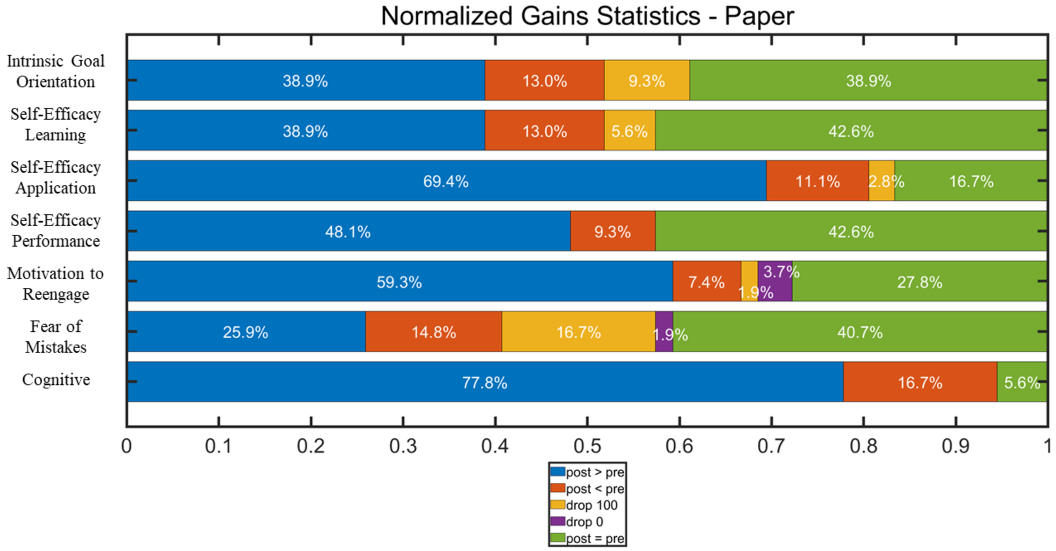

Figure 9: Normalized learning gains statistics: paper.

Appendix F   Normalized Learning Gains Histogram Plots

Performing the calculation outlined in Eq. (1) for each learner for the affective and cognitive assessments, the distribution of the normalized change for the simulation and paper format groups are shown in Fig. 10 and Fig. 11, respectively. In Fig. 10 and Fig. 11, the histogram bars are normalized by the total number of responses, such that all the bin heights add up to 1. The average and standard deviation for the normalized change for each format group are shown in the legend of each assessment.

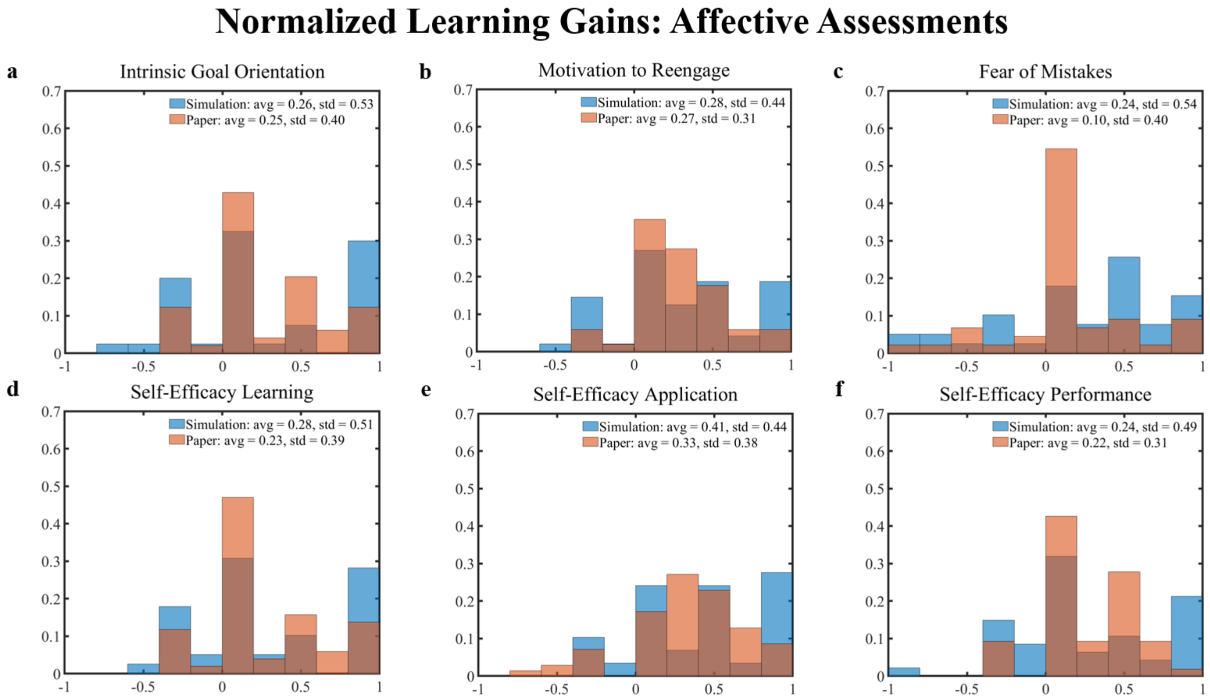

Figure 10: Normalized learning gains: affective assessments. The histogram bins are normalized so that the bar heights sum to 1.

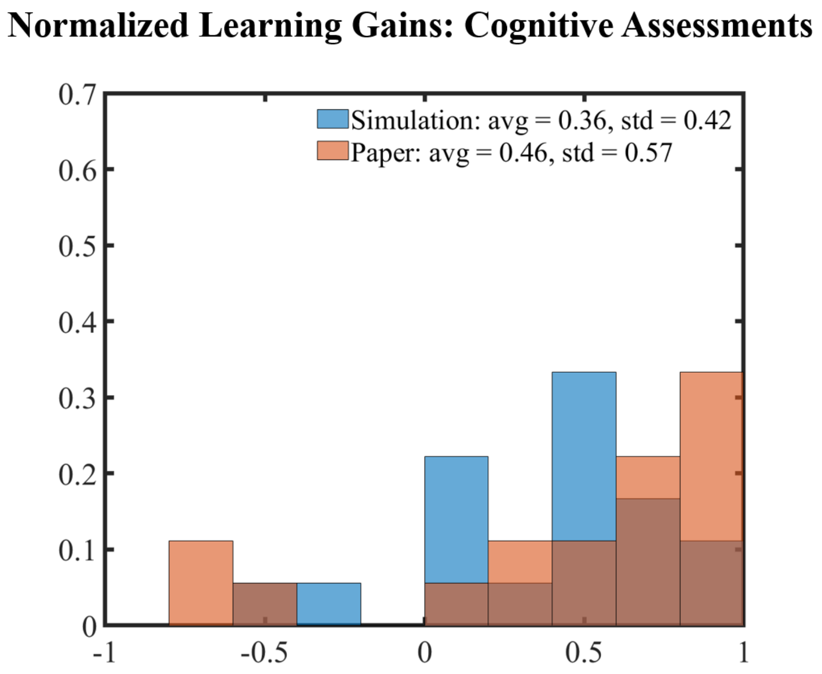

Figure 11: Normalized learning gains: cognitive assessment. The histogram bars are normalized such that the bin heights add up to 1.