Pearls Found on the way to the Ideal Interface for Scanned-probe Microscopes

Russell M. Taylor II[†]
Jun Chen
Shoji Okimoto
Noel Llopis-Artime
Vernon L. Chi
Frederick P. Brooks, Jr.

Mike Falvo
Scott Paulson
Pichet Thiansathaporn
David Glick
Sean Washburn
Richard Superfine

Department of Computer Science
University of North Carolina, Chapel Hill

Department of Physics & Astronomy
University of North Carolina, Chapel Hill

Abstract

Since 1991, our team of computer scientists, chemists and physicists have worked together to develop an advanced, virtual-environment interface to scanned-probe microscopes. The interface has provided insights and useful capabilities well beyond those of the traditional interface. This paper lists the particular visualization and control techniques that have enabled actual scientific discovery, including specific examples of insight gained using each technique. This information can help scientists determine which features are likely to be useful in their particular application, and which would be just sugar coating. It can also guide computer scientists to suggest the appropriate type of interface to help solve a particular problem. We have found benefit in advanced rendering with natural viewpoint control (but not always), from semi-automatic control techniques, from force feedback during manipulation, and from storing/replaying data for an entire experiment. These benefits come when the system is well-integrated into the existing tool and allows export of the data to standard visualization packages. For up-to-date information, see our project web page at www.cs.unc.edu/Research/nano.

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Introduction and system description

Scanned-Probe Microscopes (SPM), such as scanning tunneling microscopes (STM) and atomic-force microscopes (AFM), do not produce 2D images like optical microscopes. They use a very sharp tip to probe the surface of a sample under study. The tip can be positioned very precisely (within the radius of an atom), and reports the height at its current position. The tip is scanned in a raster pattern across the surface, producing a 2D array of heights (and other measured properties). Also, the tip in an AFM

[†] Contact Author: CB #3175, UNC, Chapel Hill NC 27599-3175. (919) 962-1701 taylorr@cs.unc.edu

can be pushed down on the surface, scraping it. This allows the AFM both to image and to modify.

Our nanoManipulator (nM) system provides a virtual environment (VE) interface to SPMs. The system provides an intuitive interface that hides the details of performing complex tasks using an SPM. It takes the 2D array of heights, tessellates with triangles, and uses a graphics supercomputer to draw it as a surface in 3D. The system uses a force-feedback device to allow the user to directly control the lateral motion of the SPM tip, using it either to feel or modify the surface (see figure 1).

Figure 1: Physics Graduate Student Scott Paulson uses the nanoManipulator to examine a tobacco-mosaic virus particle.

Earlier papers describe the nM implementation in some detail ([Taylor93] [Taylor94D] [Finch95]) and results obtained using the system in particular science experiments ([Taylor94S] [Falvo95] [Falvo97]). This paper focuses on the visualization and control techniques that have produced actual scientific benefit.

Useful features and lessons learned

During the course of this project, we have found that many aspects of the system have provided scientific insight or capabilities that allow new and fruitful types of experiments. We list specific examples of the type of insight gained by the addition of each technique.

VE display: pretty pictures moving naturally

We have found benefits to viewing even static data sets using the VE display system. This is hardly surprising; such data sets are rendered for publication as Phong-shaded 3D images to give the audience a good understanding of the surface shape.

"But we already have all the data"

All of the data about the surface that has been scanned is in fact available to the scientist even in a pseudo-color view from above.

In addition, the scientist can measure any feature of the data to exacting precision using standard techniques such as cross sections and statistical algorithms. The benefit of visualization comes from getting multiple naturally-controlled views of the data that lead to unexpected insights. Our collaborators had examined one data set using pseudo-color images and cross sections for months, yet discovered an important feature of the data (graphite sheets coming out of the surface) within seconds of viewing a real-time fly-over of the data set. These sheets were visible in only a few frames of the fly-over, when the lighting and eye point were in just the right position to highlight them. [Taylor93] See the color plates for images illustrating this. We think of each frame in a real-time display of the surface as a new filter applied to the data set, with the user in control of the filter parameters (viewpoint, lighting direction) through natural motions of head and hand. People are adept at understanding the structure of 3D surfaces this way, having learned this skill over a lifetime.

Sometimes the 2D *display is better*

For flat surfaces with small features, a pseudo-color view is superior to the shaded 3D view for two reasons: the pseudo-coloring devotes the entire intensity range to depth and obscures small fluctuations caused by noise in the image.

For features that are significant only for their height difference from the rest of the image, the pseudo-color image devotes its entire range of intensities to showing this difference. This is equivalent to drawing the surface from above using only ambient lighting with color based on height. Any 3D shading of the image uses some of this range to accommodate the diffuse and specular components at the expense of the ambient component.

This shift from ambient to diffuse/specular is a shift from displaying height to displaying slope (angle is what determines the brightness of the diffuse and specular components). This is fine for a noise-free image, but real-world images contain noise. For SPM images, a flat surface has the highest percentage of noise as a fraction of feature size. The noise causes fluctuations in illumination of the same magnitude as those caused by features, sometimes completely obscuring them.

In summary, we have found that small features on very flat surfaces are better seen using standard pseudo-color display (and are sometimes imperceptible in a 3D display). Small features on surfaces with other height variations are better brought out using specular highlighting of a 3D surface (and are often imperceptible in a 2D display). We have found this both when making patterns on photo-resist and when etching lines into thin metal films. The nM now provides both the 2D and 3D views simultaneously, each updated live as an experiment progresses.

New microscope control techniques

The nM system augments not only the display of the data from the SPM, but also the control techniques available to the scientist using the instrument. Direct control and natural observation have allowed mini-experiments and semi-automatic computer control of the tip to provide what we call virtual tips.

Mini-experiments

Using the nM, the experimenter can directly, immediately and naturally control the parameters of an experiment and can directly and immediately observe its results. This allows a mode of experimentation consisting of a sequence of mini-experiments with immediate feedback. The scientist can direct the exploration continuously and make impromptu changes to the viewing parameters and experimental plan between each mini-experiment.

This mode of operation enabled a series of experiments that led to the discovery of a process by which voltage pulses from an STM tip modify the surface. The tip welds itself to the sample after a pulse and is then drawn back until breaking free. [Taylor94S] Around 300 mini-experiments were performed and analyzed in four 5-hour blocks to determine the range and frequency of results possible; the time taken for this many mini-experiments using conventional methods would have been prohibitive.

Virtual tips: use the right tool for the job

An AFM has only the tip to modify the surface. This tool is like an ice pick that can be dragged over the surface with different amounts of force. This is not always the best tool for the job, so we use semi-automatic control over tip motion to provide *virtual tips* for the scientist to use.

Sewing machine: When trying to form a very thin line in a thin surface film, lateral scraping of the tip causes large piles of material to build up at the end of the scrape. This scraping can also cause the film to peel off the substrate. To solve this problem, we have implemented a *sewing-machine* tip that acts much like the needle on a sewing machine. The tip pulls back from the surface while moving laterally, punching down into the surface at regular intervals along its path over the surface.
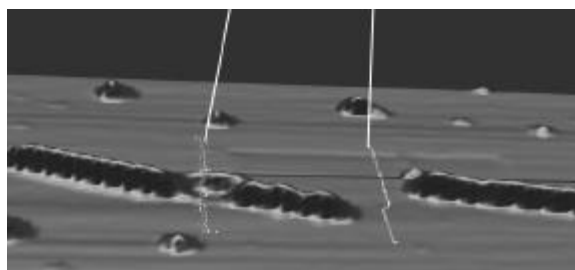
Whisk broom: Extended cylindrical structures like tobacco-mosaic virus particles and carbon filaments tend to bend and even break when the tip is moved across them in an attempt to move them. The ideal tool to move such structures might be a spatula or whisk broom. We have implemented a virtual *whisk broom* tool that rapidly sweeps the tip back and forth between two endpoints which follow the user's hand motion (see above). This rapid motion pushes each part of the cylinder forward slightly by running along its length. We have found this to be very effective in translating and rotating extended structures without damaging them.

Vibrating/contact: An AFM typically operates in one of two modes, *contact mode* or *vibrating mode*. Contact mode is described in the introduction, where the tip scrapes along the surface. Vibrating mode oscillates the tip at its resonance frequency (around 100kHz) and pushes towards the surface until the amplitude of oscillation is reduced to a fraction of its value away from the surface. Vibrating mode does not scrape the surface like contact mode, so it provides damage-free scanning on more surfaces.

The standard interface for AFMs requires that the tip be pulled away from the surface when switching from contact mode to vibrating mode, or vice-versa. This means that experiments must be performed in one mode or the other, since re-engaging the tip causes lateral position shifts.

The nM interface allows switching between contact and vibrating modes without retracting the tip. [Finch95] This allows a wider range of interaction forces between imaging and modification. This has allowed us to perform modification experiments on tobacco-mosaic virus particles and extended carbon fibers.

The positioning elements in the microscope undergo a sharp jump during the transition from one mode to the other. This results in a transient offset where the apparent surface height jumps and then relaxes to its new height over several seconds. This is compensated for automatically by the nM, avoiding what would otherwise be sharp force discontinuities as the user goes from feeling to modifying the surface. [Finch95]

Force feedback during manipulation

The force feedback component of our system has always been exciting to the scientists on the team; they love being able to feel the surface they are investigating. However, it is during modification that force feedback has proved itself most useful, allowing finer control and enabling whole new types of experiments. Force feedback has proved essential to finding the right spot to start a modification, finding the path along which to modify, and providing a finer touch than permitted by the standard scan-modify-scan experiment cycle.

Finding the right spot

Due to time constants and hysteresis in the piezoceramic positioners used by SPMs to move the tip, the actual tip position depends on past behavior. The location of the tip for a given control signal is different if it is scanned to a certain point than if it is moved there and left constant. This makes it difficult to plan modifications accurately based only on an image made from scanned data.

Position when scanning

Position after being held still for several seconds
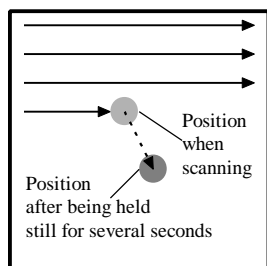
Force feedback allows the user to locate objects and features on the surface by feel while the tip is being held still near the starting point for modification. Surface features marking a desired region can be located without relying only on visual feedback from the previous scan. This allowed a collaborator to position the tip directly over an adenovirus particle, then increase the force to cause the particle to dimple directly in the center. It also allowed the tip to be placed between two touching carbon filaments in order to tease them apart.

Finding the right path

Even given perfect positioners, the scanned image shows only the surface as it was before a modification began. There is only one tip on an SPM: it can either be scanning the surface or modifying it, but not both at the same time. Force feedback during modification allows one to guide changes along a desired path.
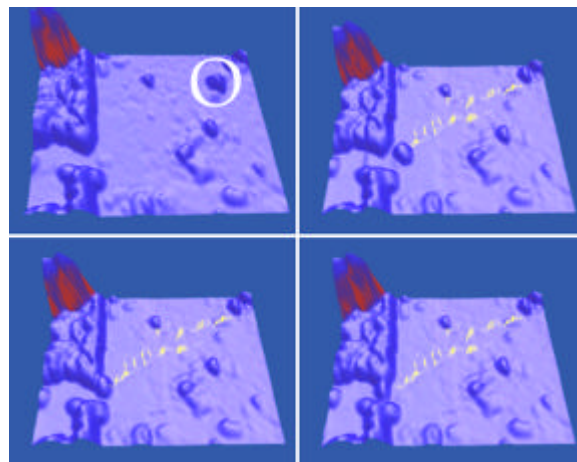

Figure 2: In this sequence of images from left to right, a 15nm gold ball (circled) is moved into a test rig. Force feedback is used to feel as the ball is pushed and to determine when it has slipped off the tip.

Pushing bags of Jell-O across a table in the dark with a screwdriver without breaking them: Figure 2 shows force feedback being used to maneuver a gold colloid particle across a mica surface into a gap that has been etched into a gold wire. This gap forms a test fixture to study the energy states of the ball. The colloid is fragile enough that it would be destroyed by getting the tip on top of it with modification force or by many pushes. This prevents attempts to move it by repeated programmed "kicks". Force feedback allowed us to tune the modification parameters so that the tip barely rode up the side of the ball while pushing it, and allowed the guidance of the ball during pushing so that only a dozen or so pushes were required.

Ring of gold: Force feedback was also used to form a thin ring in a gold film. A circle was scraped to form the inside of the ring, leaving two "snow plow" ridges to either side. By feeling when the tip bumped up against the outside of the outer ridge, another slightly larger circle was formed. This formed a thin gold ring on the surface.

A light touch: observation modifies the system

When deposited on the surface, carbon tubes are held in place by residue from the solution in which they are dispersed. On some surfaces, the tubes slide freely once detached from the residue until they contact another patch of residue or another tube. Even the light touch of vibrating-mode scanning causes them to move. By using only touch mode and switching between imaging and modification force, we have been able to move and re-orient one carbon tube across a surface and into position alongside another tube. Once settled against the other tube, it was stable again and we could resume scanning to image the surface. Force-feedback and slow, precise hand motion ("haptic imaging") allowed us to find the tube at intermediate points when we could not scan. The fact that the surface cannot be imaged at intermediate stages prevents this type of experiment from being performed using the standard scan-modify-scan cycle. See the color plates for an image of a carbon tube that is partially attached to the surface.

Storing the data for the entire experiment

If it isn't in the lab notebook, it didn't happen: An experiment is performed once, but may be analyzed many times. During analysis, questions often arise that were not in mind during the experiment itself. The lab notebook kept during the experiment

is used to help answer those questions, so the notebook must be as complete as possible.

The nM stores all data from the microscope to disk, storing the time with each message. This allows later re-play of the complete experiment from any point of view, at any scale or speed. In this way, the scientist can view the same experiment in many ways. Because of this, we don't rely on only the snapshots taken and things noted during the actual experiment.

Such replay has revealed events in past experiments that were not noticed during the experiment itself. In one case, a carbon tube was being pushed end-on towards another tube. Replay revealed that for a brief period in the middle of the experiment, it was actually pushed up on top of the other tube before sliding off. Stored images of the start and end positions missed this intermediate event. In another experiment, a carbon tube had a defect that the experimenter misinterpreted as an SPM tip artifact. Upon later reflection, the experimenter realized that the artifact had rotated with the tube, which would not be the case if it were due to the tip. Once this realization was made, the scientist went back through the experiment and was able to determine that in all but one case, the tube slid over the surface rather than rolling. In the case where it rolled, the tube had lifted free of the surface and jumped to another location before landing.

Keeping a log of the entire experiment also means that all data is available when new data analysis techniques are found. It is not necessary to run a new set of experiments to gather new data for comparison. This was useful to us when we began to use the CORE-based image analysis software to locate the center of tobacco-mosaic virus and carbon tube particles that had been bent. [Falvo97] This allowed us to fit the curve for a bent virus to a beam equation, enabling us to determine its ratio of stiffness to surface adhesion.

The nM stores not only the scan data, but also traces all steps when the user feels or modifies the surface. During these events, we can collect not just height information, but also lateral force and feedback parameters. This allows us to answer questions later regarding the stability of scan or amount of force needed to modify a surface or push an object. These traces have been used to explain the behavior of carbon tubes as the tip was pushed across them.

Analysis tools and interoperability

Two pitfalls into which the computer-science half of the team has fallen repeatedly are underestimating the need for analysis tools and the need to integrate with existing systems and overestimating the amount of polish needed to make a tool useful.

A lesson we learn over and over again as we develop new systems (such as the nM) is that providing the real-time, shaded 3D view of the surface should only be done *in addition to* the existing 2D representation with all of its analysis tools.

"Don't break what we have to give us the new"

In our most recent implementation, we have allowed the commercial (Topometrix) and nM interfaces to the microscope to operate at the same time, cooperatively. All of the existing data analysis tools, scan location changes, and parameter adjustments on the commercial interface function while the experimentation and 3D viewing is operating. This not only allows the scientists to work the way they are used to working, but keeps us from having to re-implement features already present on the commercial software. We do not yet have the ability to push the data

from the stored experiments back to the commercial interface; this still hinders the analysis performed by the scientists.

"Just give us the data!!!!!"

We have built analysis tools to perform specific tasks for the scientists (for example, computing surface curvature, displaying cross sections of the data or the trace of tip motion and other data during a modification). We often spent weeks designing just the right interface to each of these new data types, connecting them into the system. Each time, the scientists were asking "can't you just give us an ASCII file?" To them, getting the data – in any format – was an infinite improvement; cleaning up the presentation could wait.

We now provide output of the trace along the tip trajectory during each modification event, recording all of the data sets (height, the Z control signal, lateral deflection). This produces a trace of x, y, z, etc. along s (the path). These can be imported into data analysis packages and spreadsheets to do analysis. This allowed us to see the motion of carbon tubes within the middle of a push, and the force needed to pull them free from the surface.

Conclusions

Our system was designed within the paradigm of making the system invisible and allowing the scientist to interact directly with the underlying object of study. This paradigm extends to control of any instrument whose interface is either indirect or unnatural for the user but that deals with objects (such as surfaces) that are familiar to the user. This work has shown that the computer can act as effective interpreter between user and instrument, increasing the usefulness of the instrument.

Acknowledgments

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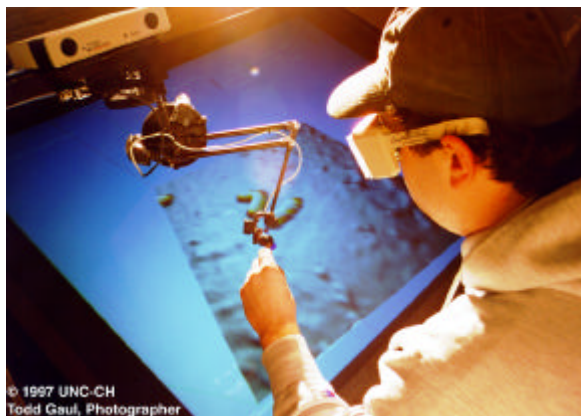
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Figure 1: Physics Graduate Student Scott Paulson uses the nanoManipulator to examine a tobacco-mosaic virus particle.

Whisk-broom virtual tip being used to sweep a section of tobacco-mosaic virus across a surface. The tracks on the surface indicate the path of the tip, which oscillates between one side and the other as the two vertical lines are swept over the surface.
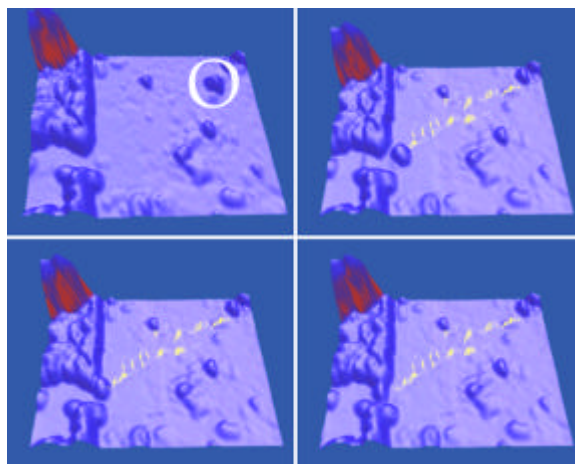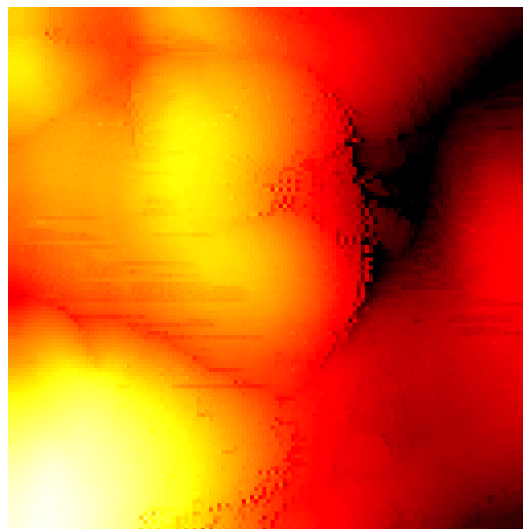

Figure 2: In this sequence of images from left to right, a 15nm gold ball (circled) is moved into a test rig. Force feedback is used to feel as the ball is pushed and when it has slipped off the tip.

Pseudo-color image of ion-bombarded graphite surface. The black-body radiation spectrum shows height. While large features are obvious, subtle detail in both the bright and dark areas is lost.
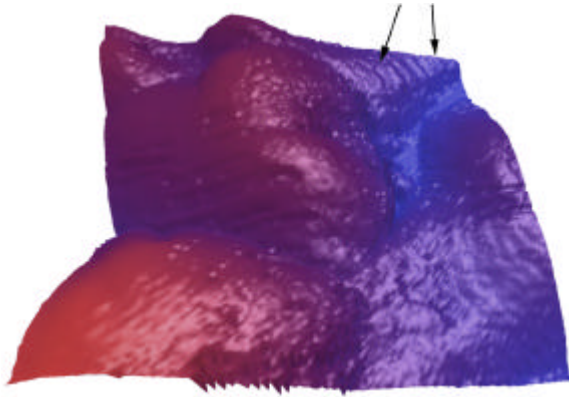
The same data set as above drawn using directional illumination of a 3D surface. Pseudo-color displays height; higher areas are red and lower areas blue. From this particular viewpoint, specular reflection reveals a regular pattern of diagonal stripes caused by layers of graphite sheets poking out of the surface.
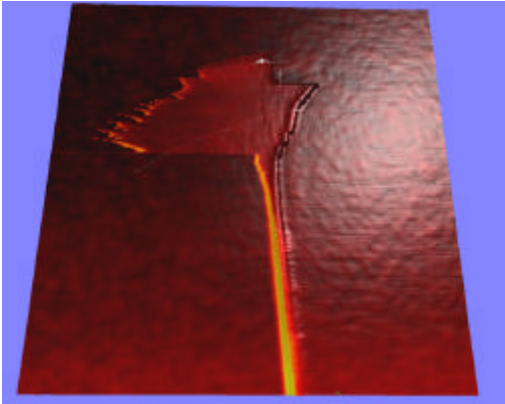

Image of a carbon tube shifting during scan. Height comes from the scan as it went to the right, color from the scan as it went to the left. The bottom half of the tube is stable, but the top half is pushed back and forth by the tip as it scans.