Scanning Tunneling Microscopy

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The invention of the scanning tunneling microscope was a singularity event in the field of surface science and condensed matter physics. The ability to visualize individual atoms in an atomic structure was a huge step forward in experimental development, one for which the inventors were awarded the Nobel Prize in Physics in 1986. While a groundbreaking development, the Scanning Tunneling Microscope is conceptually simple device which exploits both quantum mechanics and conventional mechanics in its operation. This paper will explore the scanning tunneling microscope, with a brief review of the history behind the development, then move on to discuss the physics and the art behind the use of STM, important developments made since its discovery, and where this technology is available to UTK students in the greater Knoxville area.

HISTORY

Late in the evening of March 16, 1981, Gerd Binnig, Heinrich Rohrer and a small team of experimenters held their breath as they turned on their experimental apparatus. The goal of their experiment was to demonstrate vacuum tunneling, the ability of electrons to penetrate a finite potential barrier into a distinct electronic state, for the first time. They held their breath out of a desire to avoid vibrating the delicate apparatus, but also because, if successful, this would be the demonstration of the the key invention required to complete the patent they had filed in January 1979[1] years outlining the operation of the "Scanning Tunneling Microscope"[2]. Their experiment was a success[3], and it was short work to create the fully operational STM device first reported in 1982[4], which successfully acquired surface topological data of $CaIrSn_4$ and Au surfaces. The impact on the scientific community took some time to settle in, but by the time the last doubts about the technique were cleared up with the publication of the surface reconstruction of Silicon (figure (1))[5], STM was already being heralded as deserving of a Nobel Prize.

The pursuit of scanning tunneling microscopy began as a series of discussions on the study of surface inhomogeneities and impurities, and a desire to study these on a local scale, as these types of concerns were of increasing importance to miniaturization of electronic devices[2][6]. Heinrich Rohrer and Gerd Binnig, employees of IBM in Zürich, were engaged in the study of the growth and electronic properties of insulating materials. It was Binning who brought the idea of vacuum tunneling to the table[2], and the two thought that the construction of the STM seemed like a relatively straightforward concept. Many were working on similar developments, but there was little published scientific literature. In fact, the development seemed so straightforward, that Binnig and Rohrer were surprised that no one had yet done it - the development did not require new fundamental insights, or new types of materials[6].

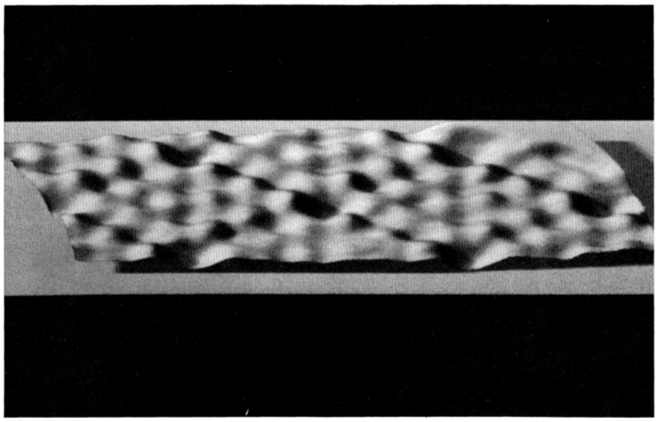

FIG. 1: The processed image of the surface reconstruction of Silicon. The reconstruction of the Si(111) surface was critical to the acceptance of STM as an experimental technique by the larger community, as attempts at structural determination of the Si surface from other experiments had largely produced conflicting results[5]. The real-space construction of this surface unambiguously determined the principal structural features. Figure from [2]

PHYSICS BEHIND THE OPERATION

The basic principles of scanning tunneling microscopy are relatively straightforward. The discussion has a good starting place in the concept of the local probe. The definition of a local probe relies mainly on the distinction of a direct interaction between the object being studied and the probe itself. In STM, a scanning probe is brought very close to the surface of the sample, such that the electronic wave functions of the tip and the sample overlap. The scanning probe is considered local as it is directly contacting the surface of the sample, and able to transfer electrons. In this configuration, there is a finite distance at which the electrons in the tip and the surface will repel, and also a distance at which they will attract. When the probe is in this equilibrium state, the resolu-

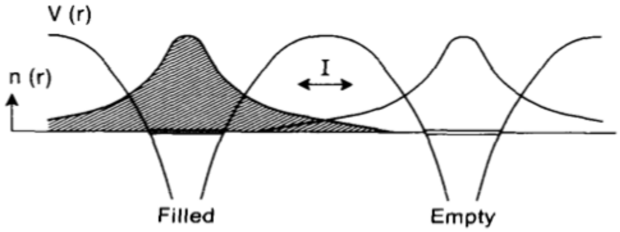

FIG. 2: Demonstration of wave function overlap between empty and filled electronic states. The electrons in the filled state have a finite probability of moving into the empty state. Figure from [2]

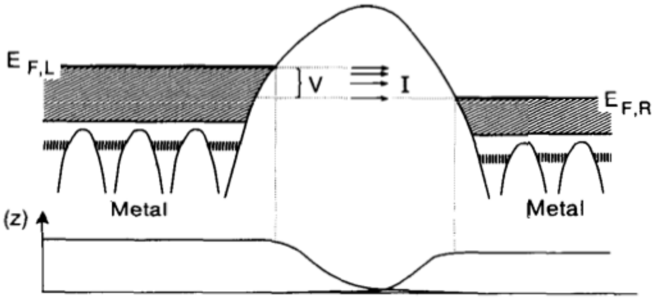

FIG. 3: Top: Difference in fermi energy giving rise to acceptor and donor states between the tip and sample. The tunneling current is created by applying a voltage to direct electrons from the higher fermi energy state to the lower fermi energy state. Bottom: electron density as a function of distance. Figure from [2]

tion of the local probe is determined by the local probe size (r), distance from the object under study (d), and the decay rate of the interaction between the probe and the material under study. If the range of the interaction is approximated as an exponential, $exp^{-x/l}$, where l is the effective decay length, a good approximation for the resolution of the probe is found to be:

$$f = A\sqrt{(r+d)l} \tag{1}$$

where A is of order 1. In this case, for f to be of the order of atomic resolution, d, r, and l must all be of atomic size[6].

In STM, the exponentially decaying interaction identified in the previous paragraph is understood as the wave function overlap of the empty and filled electron states between the sample and the scanning tip[6]. The overlap of these wave functions provide a finite probability that the electron will be able to tunnel from one state to another if an external force is applied, exploiting the concept in quantum mechanics where electrons that are incident on a finite potential barrier will not be reflected, but have a finite probability of tunneling through the barrier to be found on the other side[7]. The potential barrier in this case is the vacuum separating the sample surface and the STM tip. When the tip and the sample are brought close enough together, the wave functions will overlap, and when a voltage is applied, electrons will flow between the tip and the sample, producing the tunneling current. The tunneling current decays exponentially as the tip and the sample are moved apart, with a decay length $l(nm) \approx 0.1\sqrt{(\phi_{eff})}$ where ϕ_{eff} is the tunnel barrier between the two (commonly, ϕ_{eff} is the average of the sample and tip work functions when one considers electrons located at the Fermi energy). For most materials that are studied with STM, the value of the characteristic decay length of the interaction is close to $0.05nm$, which ensures that the tunneling current is mainly imparted to or from the sample from the front-most atom on the scanning tip[6]. The tunnel current through the barrier is approximated:

$$J_T \propto exp^{-A\Psi^{1/2}s} \tag{2}$$

where $A = (\frac{8\pi m}{h})^{1/2}$, Ψ the height of the potential barrier, s is the distance between the sample and the tip, or the effective size of the tunnel barrier[4]. The standard work functions are of the order of a few eV, giving rise to a tunneling current on the order of nanoAmperes.

The traditional STM is constructed with a tip mounted on a set of piezoelectric drives to which the voltage is applied (see figure(5)). Piezoelectric drives are a natural choice for use in STM, as their size is directly related to applied voltage, and they are able to quickly respond to changes in voltage, providing reproducible displacements with precision at the picometer level[6]. A control unit supplies voltage to the piezo drive situated in the direction of the intended scan (typically the z direction), with the voltage feedback set to maintain a constant tunnel current, which will move the tip up and down in response to surface variation as the surface is scanned. Aptly, this most common mode of operation is known as *constant current mode.* This allows the STM to map out the surface topography of the sample while the STM scans in the XY plane in a raster pattern, as shown in figure(6)[2]. Another mode, described as "constant height", maintains the height of the STM tip above the surface constant, resulting in a continual modification of the tunneling current as the scan is completed.

It is important to emphasize here that the position of the probe represent *contours of constant tunnel current*, which are then related to real systems in the material, frequently the local density of states ($LDOS$)[2]. As the tip scans the surface, maps of differential tunneling conductance are acquired ($G = dI/dV$) at all points (x, y) along the surface scanned. $(E = eV) \propto G(V)$, which results in a plot of the electronic LDOS[9]. The different regions of the LDOS can be probed by changing the tunneling current, and comparing the different scans. As a

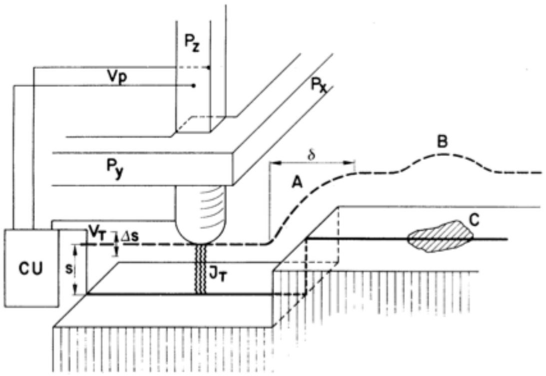

FIG. 4: Canonical STM setup, as first described by Binnig and Rohrer. The piezo drives P_x, P_y, P_z scan the tip across the surface driven by piezo voltage V_P, while the control unit (CU) supplies the tunneling voltage V_T to create the tunneling current J_T. In constant height mode, the distance s of the vacuum gap is maintained at all times, while in constant current mode, the gap s is allowed to vary, and this δs is the mapping of the surface topology directly. Figure from [4]

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consequence, both the surface topography and the LDOS can be collected at the same time, as shown in figure (7). Because of the nature of electrical conductance, the STM is blind to insulating materials, as these materials have no available electronic states in the band gap. To gain insight into the atomic nature of insulating materials, one must look to techniques like atomic force microscopy.

ART BEHIND THE OPERATION

Many who perform STM measurements will make reference to STM as being and art as well as a science. The process of performing STM measurements typically starts with a rough scan of a large surface area of the sample of interest, looking for spaces that are clear of surface impurities, undesired defects, and are relatively clean otherwise. Once an area is found in this rough scanning scheme, a finer scan of a suitable area is made, and it is from here that most of the measurements are done. Issues that frequently arise in STM include noise and impurities in the system, which must be carefully studied. For example, apparent periodicities in the structure may be attributable to noise, and typically the tip is rotated with respect to the surface normal and the system is further studied. If the periodicity does not move relative to the surface, then the feature is likely noise. If there is a notable change, then the periodicity may point to a real effect in the material, and requires further study.

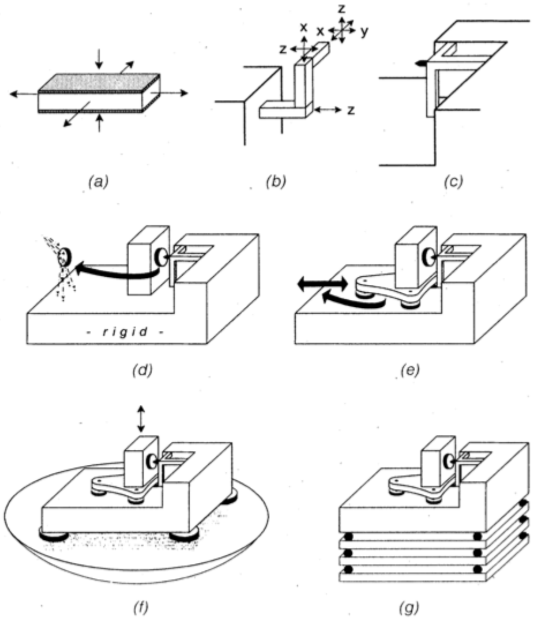

FIG. 5: Schematic STM device. (a) shows the response of a representative piezo drive to applied voltage, and (b) shows the construction of the piezo drive commonly used. (c) shows the piezo drive as an assembled unit. (e) Shows the positioning of the sample relative to the tip. In early experiments, the sample was moved toward the tip using piezoelectric positioners. Frequently, this is now done with electronic motors driving the tip position relative to the sample until close approach, at which point micropositioners and then computer algorithms take over. (f) The first STMs used superconducting magnetic levitation for vibrational isolation. This approach was used for some three months, but then discarded in favor of the easier, and significantly cheaper, vibrational isolation unit shown in (g), which consists of vacuum compatible rubber spacers between metal plates. Figure from [2]

The tips used in STM must be very carefully prepared. The most stable configuration is one that is narrowed down gradually to a size of one to three atoms at the very front of the tip, but is not long and narrow. The whole unit must be free from vibration, and long narrow tips are easily excited by thermal vibrations[4]. Other important concerns in the setup of an STM apparatus include the vacuum, which must be quite good (of the order of 10^{-11} torr to maintain the purity of the vacuum barrier between the tip and sample, and also to prevent sample contamination.

Finally, the isolation of the entire apparatus from vibration is crucial, as the scanning tip movement can be greatly impacted by vibration. Frequently, STM studies are done at night when environment vibrations are minimal, and significant investments have been made in vibrational isolation.

DEVELOPMENTS OF STM

One of the large developments of the STM technique is the use of the STM to modify surfaces when used as an atomic-scale positioner. This is possible, as the tip

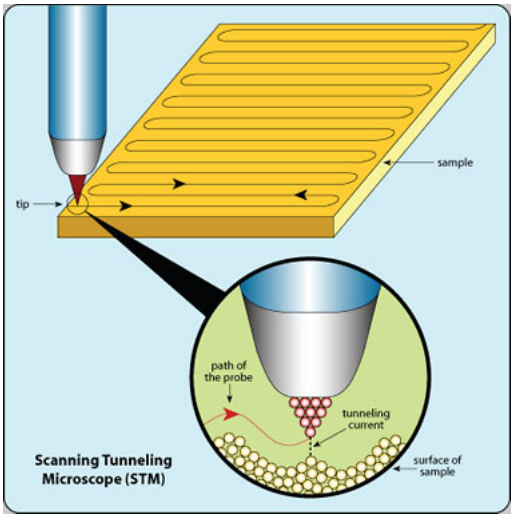

FIG. 6: The STM is scanned across the surface by applying voltage to the piezodrives in the x and y positions to create a raster pattern. The height of the scanning tip above the surface is maintained by a feedback loop to a control unit to provide a constant tunneling current. Figure from [8].

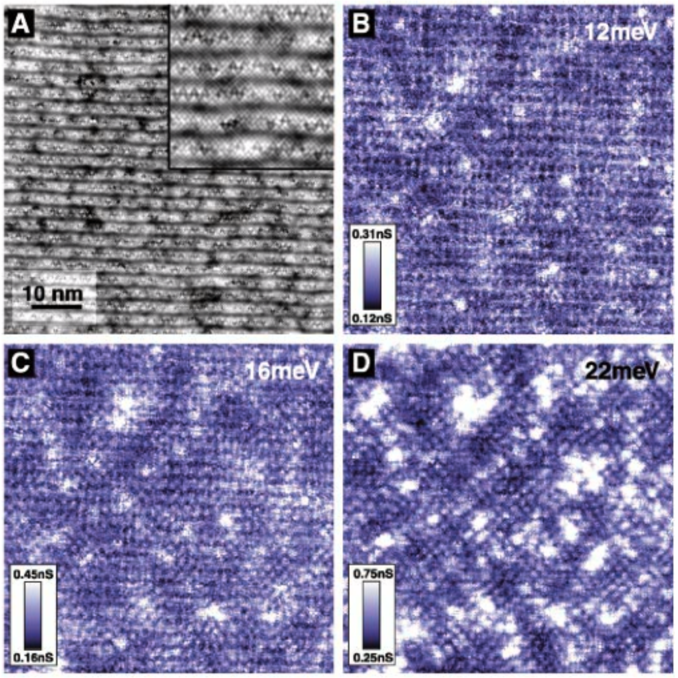

FIG. 7: (a)Topographic map of a 600x600$\mathring{A}$ area of $Bi_2Sr_2CaCu_2O_{8+\delta}$. (b)-(d) LDOS plots at several energies. A checkerboard type spatially modulated pattern is observed in all LDOS plots. Figure from [9]

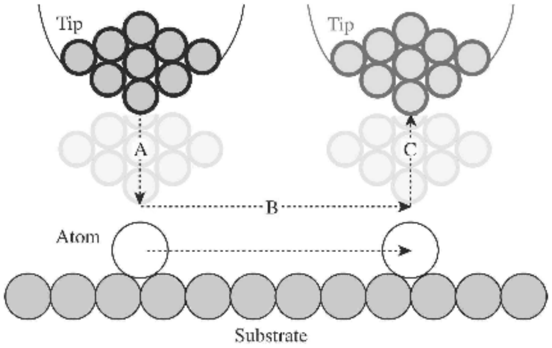

FIG. 8: Illustration of the principle of atom movement with the STM. The Xe atom is "lifted" or "pushed" across the surface of the metal substrate a distance c, at which point the tunneling current is adjusted to reposition the atom. Figure from [10].

of the STM exerts a combination of Van der Waals and electrostatic force on the surface atoms of a sample. By adjusting the position and voltage on the tip, it is possible to exploit these interactions to pull an atom across the surface of the sample with the microscope tip (as illustrated in figure(8)). This allows for the creation of designer setups, as shown in figure(9), and is hoped to provide avenues for precisely designed miniature devices[10]. The force required to move an atom on a substrate was recently measured in the 10's to 100's of piconewtons, but this number is highly dependent on the atom being moved and the surface[11].

The first steps in device miniaturization realized by STM have been taken by several groups, and are illustrated in particular by the work of the Yazdani group at Princeton. The group at Princeton has constructed galium-arsenide semiconductors, which were then doped with manganese on the galium site, with the STM performing this substitution, a process that hasn't been reproduced on the macroscale. What was developed was a nanoscale semiconductor that had magnetic properties from the inclusion of the manganese[12].

Another particularly interesting development in STM is the use of fourier transforms of the real-space local density of states images. This technique allows the measurement of the topographic imaging that is standard with STM techniques, the measurement of real-space local density of states information, and then the momentum-space information on wave functions and scattering processes[9]. An example of a study using this technique was performed by J. Hoffman and colleagues on the cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$, where real space local density of states information was fourier transformed to show that the scattering vectors in the sample had an asymmetric dispersion and differed in size as the local density of states was studied (see figure(7)). The periodic modulations in the LDOS are interpreted as effects from quasiparticle interference[9].

The final development to be discussed is the STM as a probe of superconducting pairs. Again, in a work done by the Yazdani group of Princeton, they used a spe-

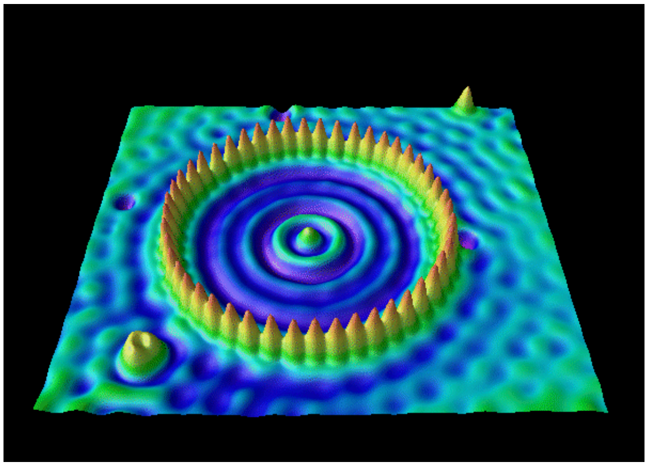

FIG. 9: "The Quantum Corral", one of the most famous atomic arrangements created with the use of STM as an atomic positioner. The image shown here depicts a circular arrangement of cobalt atoms on a copper substrate. The Bessel function like substructure is standing waves generated by the reflection of the wave functions of the copper surface electrons by the cobalt atoms. Figure from [13].

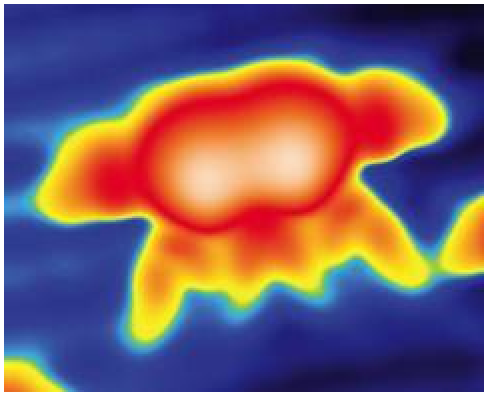

FIG. 10: Image of a manganese doped GaAs semiconductor creating with an STM. The creation of this piece paves the way for miniature devices that are capable of both storing data and performing calculations. Figure from [12].

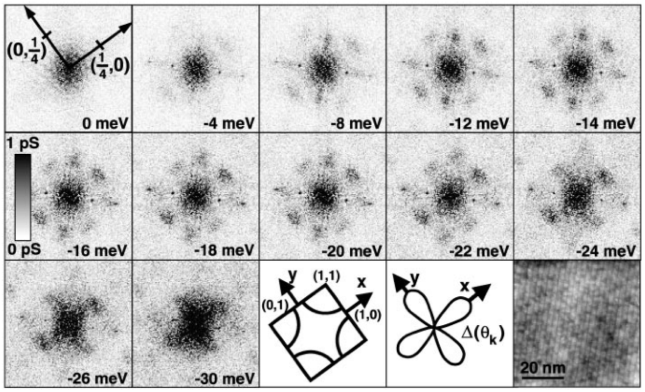

FIG. 11: Bottom - The fourier transformed LDOS plots shown in figure(7), along with the orientation of the $\vec{q}$ vectors, Fermi surface, and topographic images. The change in wave vector length with energy is inverse between the $\vec{q}$ in the $(\pm\pi,0),(0,\pm\pi)$ direction compared to the $(\pm\pi,\pm,\pi)$ directions, and also with different dispersions. Figure from [9].

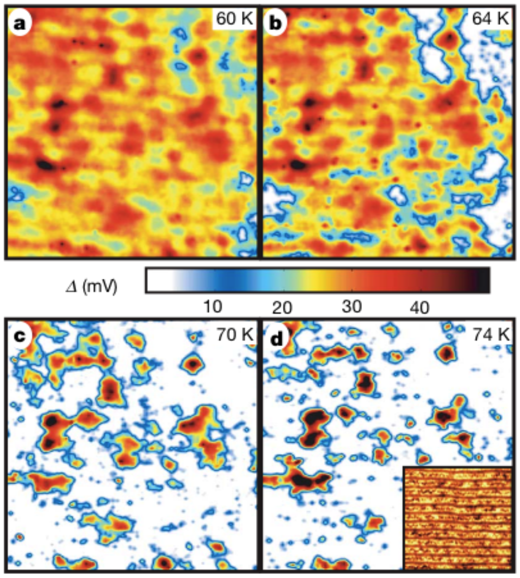

FIG. 12: Details on the evolution of the superconducting gap in overdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$. This particular sample as a T_c of 65K, and temperature at which the experiment was conducted are shown in the upper right of each figure. System topographic map is shown in the inset to figure d. Regions exhibiting what is explained as a superconducting gap are clearly visible up to 74K. Figure from[14]

cialized STM to probe the LDOS of a fixed region of a cuprate superconductor ($Bi_2Sr_2CaCu_2O_{8+\delta}$) as a function of temperature, and repeated this for many different doping levels. By interpreting the maximum values of the local conductance as attributable to the presence of a superconducting "pairing state" located at a particular position in *(x,y)* space, what they found was that superconducting pairing regions were present at a temperature above the superconducting critical temperature, and more spatially uniform as the material was cooled below the transition temperature, as shown in figure (12)[14]. There are many implications of this particular finding, not the least tantalizing of which is the possibility to create exotic superconductors based on relocation of these pairing states.

AVAILABILITY IN THE AREA

In the Oak Ridge Area, there are several scanning tunneling microscope facilities that are available for use. At the Center for Nanophase Materials Science[15] on the Chestnut Ridge site at Oak Ridge National Laboratory, there is a full scale user program that solicits applications for use of the equipment in nanophase material fabrication and characterization. Specifically to STM, there are several set ups that offer STM capability, two of which provide in-situ material fabrication and surface analysis with a molecular beam epitaxy unit connected to an STM setup in an ultrahigh vacuum environment. There are also ultrahigh vacuum cryogenic systems that provide the ability to image and manipulate surfaces at varying temperatures, or high magnetic fields *(under development)*[16]

In the condensed matter physics department at the University of Tennessee, the laboratory of Dr. Hanno Weitering possesses an ultra high vacuum containment unit that has molecular beam epitaxy, X-Ray Photo Emission Spectroscopy, low energy electron diffraction, and variable temperature STM capabilities. There is also capability to perform *in-situ* cleaving of samples, as well as a sophisticated control system and data analysis setup. All of these instruments are contained in a single ultrahigh vacuum system, allowing for material growth, sample preparation, and characterization without exposing the sample to the outside environment. This provides a clean setting for the experiment from construction to characterization, and ensures that the sample defects and impurities are low[17].

CONCLUSION

This paper has presented a brief history of the scanning tunneling microscope, discussed the physics behind the operation, as well as highlighting some of the important discoveries made with STM, and some new developments that have grown out of the use of the STM in the past two decades. Location of experimental equipment was provided to encourage the reader to further investigate at close range this conceptually simple, but scientifically profound technique first hand.

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