Scanning tunneling microscope automation

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A computerized system for scanning tunneling microscope control, data acquisition, and display is presented. It is based on the IBM Personal Computer Model XT or AT. An IBM Data Acquisition and Control Adapter card is used for the PC to control the electronic equipment and to measure the voltages applied to the three STM piezoelectric elements and the tunneling current. An IBM Professional Graphics Controller card is used for real-time display of the STM "images." The software has been designed in a modular way to allow the replacement of these cards and other improvements to the equipment. A discussion of performance (scanning speed and size of images) is included. Some image analysis and display tools are included for *a posteriori* image processing.

1. Introduction

The scanning tunneling microscope (STM) has been demonstrated to be an efficient and reliable tool for the observation of surfaces with atomic resolution [1, 2]. The recent improvements in STM design have proven that it is not only an ultrahigh-resolution microscope but also an instrument easy to build and to operate. For a review of the state of the art, see [3]. This microscope, compared to the different types of electron microscopes, is weakest in data display. The major challenge that scanning tunneling microscopists face today is the development of computerized systems [4] for STM control, data acquisition, and real-time display. The next objective will be the development of image processing techniques suitable for the restoration and analysis of STM "images."

This paper describes a system set up by the IBM Madrid Scientific Center for STM control, data acquisition, and display. The work is part of a multidisciplinary project jointly conducted with the IBM Zurich Research Laboratory, the Center of Molecular Biology of the Spanish Scientific Research Council, and the Department of Fundamental Physics of the Autonomous University of Madrid, where the STM laboratory is located. The objectives of this project are applications of scanning tunneling microscopy in molecular biology and surface science.

The system (hardware and software) design takes into account the following requirements:

- It must satisfy the requirements of an STM laboratory whose equipment and researchers are evolving from the use of a manually operated microscope with analog plotter prints as unique output, to the use of a computerized microscope that includes digital image display and processing facilities.
- It must be capable of being assembled using "off-the-shelf" hardware, except for some simple electronic pieces easily built in any laboratory.
- The software has to be flexible enough to support, with only minor modifications, the replacement of critical hardware components by others with higher performance that may become available in the future.

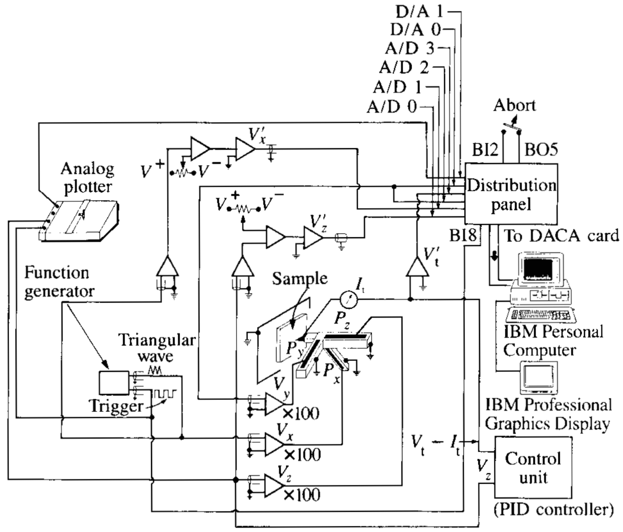

Figure 1

Block diagram of the STM control, data acquisition, and display system indicating all the equipment connections. Amplifiers labeled "× 100" are high-voltage high-gain amplifiers.

- It must be written in a high-level language (with the exception of some critical routines written in ASSEMBLER) to allow the end users to include their own routines for data analysis.

The system is based on the IBM Personal Computer Model XT or AT; it currently uses an IBM Data Acquisition and Control Adapter card for control and data acquisition and an IBM Professional Graphics Controller card for image display. Their replacement by newer and more efficient cards, and certain changes in the analog hardware around the microscope, are under consideration. The Personal Computer provides data acquisition and real-time display operations as well as certain control operations. In addition, some data analysis algorithms are also provided to allow the microscopist to take a quick look at the data that will aid in searching for sample areas appropriate for observation, as well as in selecting some images for thorough analysis in the main computer.

The large STM images are analyzed more efficiently in a mainframe. Therefore, after acquisition they are usually transferred to a large computer where image processing tools are available. The Madrid Scientific Center has developed, in the course of other research projects in the area of image processing, a number of tools for the restoration of images [5], for the analysis of electron microscope photographs in two [6] and three dimensions [7, 8], and for the display of three-dimensional objects [9], and these are now being applied to the scanning tunneling microscope images.

The next section of this article is devoted to the description of the basic hardware used in our system for STM control, data acquisition, and image display. Section 3 describes the operation of the control and data acquisition program, as well as the data analysis tools it incorporates. Section 4 presents our procedure for displaying the STM images on a high-resolution monitor in real time. We discuss in Section 5 the performance of our system in its present state and the effect that some hardware improvements will have on it. Section 6 describes a package of image processing tools that are also available in the STM control PC for performing image analysis and high-quality display *a posteriori*.

2. Hardware

The precise pieces of equipment used for control, data acquisition, and image display in scanning tunneling microscopes differ from one installation to another. Even in the same installation, the evolution of the STM techniques and the appearance of higher-performance hardware often bring about the modification of this equipment. However, the basic hardware is similar in most cases. We list below the hardware (analog and digital) actually supported by our STM control, data acquisition, and display program (see **Figure 1**).

Personal computer An IBM Personal Computer (XT or AT) is required for control, data acquisition, and display. If the STM image is directly stored in a fixed disk, 128K bytes of memory will suffice. However, if it is stored in the random access memory in order to increase the data acquisition speed, the largest amount of memory is required. An IBM 3278/79 Emulation Adapter card can be used to connect the PC to a mainframe.

Scanning tunneling microscope From the point of view of control and data acquisition, the STM consists basically of three mutually orthogonal piezoelectric elements. The x- and y-piezoelectric elements produce scanning along the x and y directions respectively by applying the voltages V_x and V_y to them. The voltage applied to the z-piezoelectric element is generated by a control unit.

Control unit A control unit is required to generate the voltage V_z applied to the z-piezoelectric element, as well as to measure the tunneling current I_t and maintain it constant. In our case, the control of I_t is performed by means of a PID (proportional-integral-differential) controller that generates the V_z potential applied to the z-piezoelectric element.

As is well known, when the distance between the tip and the sample surface varies, the tunneling current I_t also changes; the PID controller then modifies the voltage V_z applied to the z-piezoelectric element to restore the original value of I_t. In this way the voltage V_z represents the "topography" of the sample as the tunneling current I_t is maintained constant.

Data acquisition and control device Our system currently uses the IBM Data Acquisition and Control Adapter (DACA) card, although it may be easily replaced by any equivalent, though faster, card whose software support is written in ASSEMBLER callable from BASIC. The DACA card has two analog outputs with 12-bit resolution, four analog inputs, a digital output of 16 bits and a digital input of 16 bits. The analog input channels multiplex into one A/D converter of 12-bit resolution; the rate of data sampling can be as high as 17 kHz. The dynamic ranges of the analog inputs and outputs are switch-selectable: 1) from 0 to +10 volts, 2) from −5 to +5 volts, and 3) from −10 to +10 volts.

We use the four analog inputs to measure the tunneling potential V_t and the voltages V_x, V_y, and V_z applied to the x-, y-, and z-piezoelectric elements (actually, signals proportional to these voltages are measured at the beginning and end of every scan). The z-piezoelectric voltage V_z is sampled many times during each forward scan; these values constitute what we call an STM image. Connections to the A/D inputs have to be carefully made in order to avoid noise. The best solution is the use of a differential mounting with shielded twin wires. The two analog outputs are used to control the y coordinates of the tip and of the plotter pen, incrementing V_y and the base y-signal of the plotter after every scan. The digital input is used to trigger and stop the data acquisition process.

Distribution panel The IBM DACA distribution panel is used to arrange the connections between the DACA card and the electronic equipment required by the microscope.

Function generator The voltage applied to the x-piezoelectric element is a symmetric triangular wave supplied by a function generator. A square wave trigger signal, synchronous with the triangular wave and generated by the same apparatus, is used to trigger the acquisition of data and the motion of the plotter pen. This signal is connected to binary input number 8 of the DACA card (i.e., to bit 8 of the binary input).

A second function generator was formerly used to provide the voltage applied to the y-piezoelectric element. This approach had two serious drawbacks—it was very difficult to obtain triangular waves of less than 10^{-3} Hz with high stability, and scan-skew error was always introduced in the images. Instead we use the D/A output of the DACA card to control the y position of the tip by incrementing the voltage V_y by a constant amount after every scan.

Amplifiers Three high-voltage, high-gain amplifiers are needed in our microscope to apply the voltages to the piezoelectric elements. The inputs to these amplifiers are provided by 1) the function generator for the x-piezoelectric element, 2) an analog output of the DACA card for the y-piezoelectric element, and 3) the control unit for the z-piezoelectric element. These high-voltage amplifiers are not needed when more efficient piezoelectric elements are used.

Another two amplifiers with variable offset are needed for adapting the inputs of the high-voltage amplifiers that act on the x- and y-piezoelectric elements to the dynamic range of the analog inputs of the data acquisition and control adapter.

Data display devices Some kind of device is always needed to visualize the values of the z-piezoelectric voltage V_z while data are being collected. An analog x-y plotter has been traditionally used by scanning tunneling microscopists to produce hard copies of their observations. However, the slow motion of its pen sets a very restrictive limit to the scanning frequency. The use of a digital image display device allows much faster scanning. Our system supports both, an analog x-y plotter and an image display card which at present is an IBM Professional Graphics Controller with an IBM Professional Graphics Display (see Section 4 for a more detailed description).

In addition, a digital plotter is supported through the RS 232C interface to produce hard copies of the STM data once their acquisition has been completed.

3. Software

The computer program that performs the control, data acquisition, and display of the scanning tunneling microscope has been written in BASIC and compiled. It has been linked with some ASSEMBLER subroutines for the critical tasks in order to get a fast and compact executable module which works under DOS Version 2.0 or higher. It is arranged in a modular way to allow the microscopist to select the control, data acquisition, and display steps to be performed, as well as to facilitate modification of the routines as required by the coming hardware changes.

The program is organized in four well-defined parts: 1) setting of the parameters that determine the operation of the microscope, 2) STM control, data acquisition, and real-time display (the real core of the program), 3) file management, and 4) some processing tools for immediate data analysis.

• *Setting of parameters*

Before starting the data acquisition process, the program requests the following information about the experiment to be performed:

- An experiment identification name and a descriptive text.
- The sampling frequency and the number of samples per scan; this last number should be a power of two to facilitate the computation of the discrete Fourier transform (see the subsection on immediate data analysis).

- The maximum number of scans (the actual number of scans may be smaller if the experiment ends prematurely).
- The ranges of the D/A and A/D converters.
- The calibration of the x-, y-, and z-piezoelectric elements in angstroms per volt.
- A switch parameter to select whether coordinate data are given in volts applied to the piezoelectric elements or directly in angstroms.
- The initial voltage to be applied to the y-piezoelectric element (actually to the amplifier whose output is applied to the y-piezoelectric element).
- The increment applied to the y-piezoelectric element per scan (either in volts or angstroms).
- The conversion factors of the digital counts to the real values of the voltages V_x, V_y, and V_z applied to the piezoelectric elements.
- A switch parameter to select the use of the analog plotter.
- The voltage applied to the plotter to position the pen on the paper, and the voltage increment after every scan.
- A switch parameter to indicate whether real-time image display is wanted.
- Minimum and maximum pixel values used for the normalization of the displayed STM image (see Section 4).
- The type of storage (disk or memory) and the data format (character or binary).

The default values of these parameters can be obtained from a program profile, which allows the microscopist to avoid going through several menus. This profile can be modified at the end of an experiment by saving the current parameter values.

In addition, the disk file that will contain the STM image is opened and the display is initialized if these functions have been selected.

- *Control, data acquisition, and display*

During each cycle of the STM operation, i.e., each forward and backward tip scan along the x direction, the program performs the following actions:

Data acquisition trigger The status of bit 8 of the binary input (which is connected to the trigger signal synchronized with the x scan signal) is sampled at the maximum speed and each two consecutive values are compared. When a transition from 0 to 1 is detected, the program begins to acquire data.

Measurement of V_x, V_y, and V_t The voltages at the analog input channels 1, 2, and 3 are measured and stored in a matrix. These voltages are proportional to the voltages applied to the x- and y-piezoelectric elements and to the tunneling potential.

Measurement of V_z The voltage at analog input channel 0, which is proportional to the voltage applied to the z-piezoelectric element, is sampled at the desired rate during the x forward scan and its values are stored in an array.

Measurement of V_x, V_y, and V_t At the end of the scan, the voltages at analog input channels 1, 2, and 3 are measured again and stored in the same matrix. The actual values of V_x, V_y, and V_t are displayed in the PC monitor in order to check whether the experiment is running as planned.

Tip stepping along the y-direction The voltage on analog output 0 is incremented by the required amount to produce a displacement of the tip along the y direction. This is achieved by an increase in the voltage V_y applied to the y-piezoelectric element. If the voltage V_y becomes larger than the maximum allowed (or smaller than the minimum when the increment is negative), the experiment is ended.

Plotter pen stepping along the y-direction If the analog plotter is being used, the voltage on analog output 1 is increased by the amount required to increment the base y-coordinate of the pen.

Scan data storage If the STM image has to be saved in disk in real time, the values of V_z measured during the scan just completed (which are stored as elements of an array) are appended to the disk file.

Image display If the STM image has to be displayed in real time, the values of the z-piezoelectric element voltage V_z are transformed into the pixel values V_z' (see Section 4) and sent to the image display card.

Abort status The value of bit 2 of the binary input is read. If a value of 1 is found, the experiment is ended. The microscopist can set this bit to 1 by means of a switch.

The program proceeds again with the data acquisition trigger step. If the x scanning frequency has been set so high that there is no time to store and display the data while the tip is moving backward, the tip scans at least once with no data being collected and no increment to its y-coordinate. Therefore, even if the x scanning frequency is inappropriately high, the STM image is correctly acquired. However, the program tells the microscopist the maximum appropriate scanning frequency.

- *File management*

Once the experiment has been completed, the STM data and other relevant information are stored in four disk files (one of them optional) whose names are the same (the one given to the experiment) and whose extensions are different. These files are the following:

Name.HDR contains the information about the experiment. It contains the values of the relevant parameters and the other data listed in the subsection on parameter setting.

Name.XYT contains the values of the V_x, V_y, and V_t voltages at the beginning and at the end of every scan.

Name.STM contains the digital values of the z-piezoelectric element voltage collected along all the scans, i.e., the STM "image" $V_z(x, y)$.

Name.FFT contains the discrete Fourier transform of each scan. This file is created only when the Fourier transform has been computed (see the subsection on immediate data analysis).

The file with the STM image (Name.STM) can have two different data formats selectable by the microscopist:

- Character format. In this case data are stored as the integers that represent the digital values of the voltage measured by the A/D converter (numbers between 0 and 4095) in character format, separated by blanks. Therefore every single datum occupies 5 bytes. Peeking at this file with an editor, one can easily read the measured values.
- Binary format. In this case every single datum occupies a PC word, i.e., 16 bits, of which the first 4 are always 0. This format is difficult to interpret when peeking at the file but requires 2.5 times less storage space and time.

The program incorporates the possibility of converting STM image files from character format to binary format and vice versa.

- *Immediate data analysis*

Once the data acquisition has been completed, the program allows the microscopist to perform some analysis of the collected values of the z-piezoelectric element voltage V_z. It provides very significant information about the actual STM operation and therefore it is advisable to collect and analyze data from a few scans prior to the acquisition of a complete image. In particular, this analysis yields some parameters required by the real-time display routines to increase the dynamic range of the displayed data. The functions available are the following:

- *Discrete Fourier transform* (DFT) of each scan to find its frequency spectrum. This information is relevant in that it permits the microscopist to see whether there is any periodicity in the data, whether there exists any periodic noise that the system is getting, or whether the signal-to-noise ratio is too small. The DFT is computed with the fast Fourier transform (FFT) algorithm for a number of samples that is a power of 2 [10].
- *Mean value,* $\bar{V}_z$, of the V_z samples of each scan.
- *Root mean square noise* of the samples of each scan defined as $1/N\sqrt{\Sigma[V_z(x) - \bar{V}_z]^2}$, where $V_z(x)$ are the N samples of V_z collected in a scan. This value gives information about the reliability of the data.
- *Real-time display parameters* used to increase the dynamic range of the STM image displayed on the monitor. The image actually displayed is

$$V_z'(x, y) = C[V_z(x, y) - (A + Bx)],$$

where C is a scaling factor and the parameters A and B are obtained by a least-squares fit of the values $V(x, y_0)$ collected in a test scan, also taking into account that the values $V_z'(x, y_0)$ should range between a minimum (greater than 0) and a maximum (less than 255) selected by the microscopist to have a reasonably good probability that $V_z'(x, y)$ does not fall out of the range of possible pixel values.

4. Image display in real time

During the tip trace-back time, the data collected in the forward scan just completed can be displayed on a high-resolution color monitor by means of an image display card installed in the Personal Computer. Our system currently uses an IBM Professional Graphics Controller and an IBM Professional Graphics Display. Its future replacement by another display card with higher performance has been taken into account in the design of the display routines.

The refresh buffer of the IBM Professional Graphics Controller has 480 × 640 8-bit pixels and a video lookup table (VLT) with 8-bit input and 12-bit output; 4 bits are used to control the brightness of each primary (red, green, and blue). Therefore, up to 256 different colors can be simultaneously displayed. They are chosen from among 4096 possible colors (those obtained with 16 levels of red, of green, and of blue). In particular there are 16 gray levels (those colors with the same brightness in the three primaries).

A maximum of 480 tip scans can be displayed. Additional scans are either displayed replacing the first scans or not displayed (as selected by the microscopist). Up to 640 samples per scan can be displayed. If scans are longer, the microscopist must select the samples to be displayed.

The actual pixel values $V_z'(x, y)$ sent to the refresh buffer are linearly related to the z-piezoelectric element voltage by the transformation

$$V_z'(x, y) = C[V_z(x, y) - (A + Bx)],$$

whose parameters A, B, and C have been obtained from the data of a test scan. The values of $V_z'(x, y)$ should range from 0 to 255. If these values happen to lie outside this interval (for instance as a consequence of the tilt of the sample), a bit clipping, easily identifiable by the microscopist, occurs.

A color code is used by means of the VLT to optimize visual discrimination of levels. It can be checked by means of a color wedge displayed as reference when there are no more than 512 samples per scan. This color coding has been specially designed to provide the microscopist with the maximum information about $V_z(x, y)$ that is possible, according to perceptual color space considerations [11], using the actual image display card. It has been selected to be the maximum-length path in the discrete color space along saturated colors. The metric of the CIE 1976 $L^*u^*v^*$ uniform color space [12] has been used to calculate perceptual distances between colors. In the perceptual color space of the IBM Professional Graphics Controller [11], characterized by having four bits per primary, our code consists of 106 different colors along the path black-green-cyan-blue-magenta-red-yellow-white.

Because the number of colors used for coding is smaller than the number of values that V_z' can take on, several values must be represented by the same color. The number of V_z' values represented by each color is set proportional to the perceptual distance between this color and its neighbor VLT colors, in order to have a perceptually equalized color distribution which maximizes the amount of information about $V_z'(x, y)$ perceived by a standard observer.

5. Performance

The maximum size of the STM images $V_z(x, y)$ that can be collected is determined by the data format (character or binary) and the type of storage (computer memory or disk) which is used during data acquisition. In binary format, a 512 × 512-pixel image occupies 512K bytes plus 6K bytes for the values of V_x, V_y, and V_t collected at the beginning and end of every scan. A PC with 640K bytes of random access memory is thus required if images of that size have to be stored in the computer memory. If the images are stored directly on fixed disk, they may have some ten million pixels.

The data acquisition speed is limited by the piece of the equipment with the lowest performance, which may vary as the actual system configuration evolves. In accordance with the piece of hardware that is setting the speed limitation and the precise value of this limit, different image storage and display strategies can be adopted. Our software supports four different strategies determined by storage method (whether the STM image is kept in the random access memory or downloaded to disk) and the real-time or delayed display of the image.

The slowest component of our system is obviously the analog plotter, whose use must be avoided when a good data acquisition speed is wanted. Apart from it, the components with lower performance at present are the high-voltage amplifiers (about 2 kHz cutoff frequency). According to the Shannon-Whittaker theorem [13], the maximum sampling rate should be 4 kHz if there is no oversampling. This also sets a rather low limit to the linear speed of the tip.

Once these amplifiers have been removed (replacing the STM piezoelectric elements by more efficient ones), the speed limit will be set by the data acquisition and control adapter or by the image storage and display strategy, until a higher value is reached at which the control unit or the mechanical parts of the microscope will become the limiting factors.

The following is a discussion of scanning speed, in which we always assume scans of 512 samples and refer to an IBM PC-AT.

The maximum data acquisition speed that can be achieved using the IBM Data Acquisition and Control Adapter card is equivalent to a rate of 16.6 scans per second.

By storing the STM image in fixed disk without simultaneously displaying it, a rate of 21.4 scans per second (16.0 using instead an IBM PC-XT) could be achieved. If the image is displayed in real time by means of an IBM Professional Graphics Controller, the maximum rate is 12.2 scans per second, which can be improved by replacing it with a faster display.

If the image is kept in the computer memory without being displayed, the data acquisition rate may be a few hundred scans per second (depending on the actual performance of the data acquisition and control card used). Displaying the image in real time through the Professional Graphics Controller gives a speed limit of 21.0 scans per second.

Therefore, if we want the image to be downloaded to disk and displayed in real time, the IBM Data Acquisition and Control Adapter does not limit the system speed unless a much faster display card is used. On the other hand, if the DACA card is replaced by a faster one, the images should be kept in computer memory and the Professional Graphics Controller should be replaced by a faster display.

6. Image processing

Once an STM image has been collected, data are transferred for processing from the IBM Personal Computer to a large computer. We use an IBM 4381 with a Ramtek 9351 image display unit and an IBM 7350 image processing subsystem to analyze the STM data.

In the mainframe there are available algorithms for systematic and random error correction specially designed for STM images, as well as general-purpose image processing tools. The latter include geometric transformations using bilinear and cubic convolution interpolation, spatial filters, Fourier transform, frequency domain filters (including the Wiener [5] and lattice-pass [6] filters for image restoration), and correlations. There are also tools for displaying two-dimensional pictures in black and white and pseudocolor, and for representing three-dimensional surfaces seen with any orientation and illuminated from any direction [9]. Examples of this three-dimensional display are **Figures 2** and **3**, which show the STM image of an electrochemically activated platinum surface [14] seen from two different viewpoints and illuminated at different angles. Figure 2 is a top view with low-angle illumination which is very convenient for observing the surface relief, while Figure 3 presents a conventional oblique perspective view.

Most of these algorithms are highly time-consuming and/or require large amounts of computer memory, in particular those involving Fourier transforms. However, those processing algorithms that do not require too large a computer memory and that are not heavily time-consuming have been also implemented in the Personal Computer that controls the STM, in order to make a quick survey of the images just after data collection to determine whether they deserve a thorough processing in the main computer. The IBM Professional Graphics Controller is used for the display of the images.

The image processing tools available in the STM control PC include algorithms for systematic data correction, such as change of scale and correction of the drifts of the scan origin and of V_z. In particular, the subtraction of a plane accounting for the smooth variation of V_z due to sample tilt is essential to optimize the dynamic range of the displayed image. Space domain filters are available for smoothing (variable-size window averaging), sharpening (Laplacian filter), and edge detection (gradient filter using the Sobel kernels). For a more detailed description of these image processing techniques, see for instance [15].

Images can be displayed using the same color coding described in the previous section. However, a better matching of the dynamic range of data to the set of colors can now be achieved, in order to optimize the visual interpretation of the images, either based on the image histogram or done directly by the microscopist.

The STM images $V_z(x, y)$ can also be displayed as three-dimensional surfaces [16]. To facilitate the observation of the sample topography, the orientation of the surface can be chosen by the microscopist, as well as the point from which the surface is being illuminated and the relative proportions of direct and isotropic diffuse light applied.

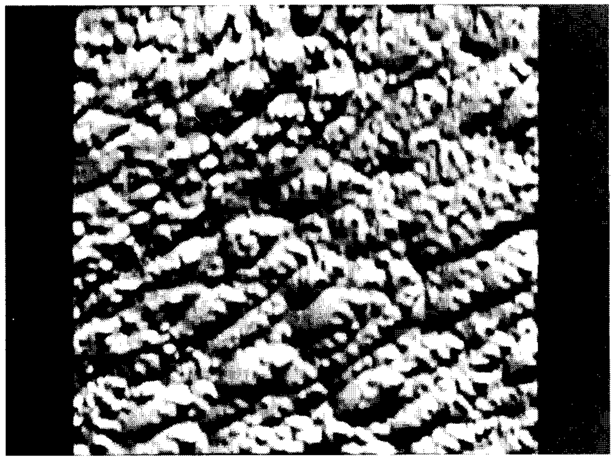

Figure 2

Top view of the STM image of an electrochemically activated platinum surface. The elevation of the light source is 20° and there is 20% diffuse light. The image has been filtered to eliminate the noise and interpolated to have the same scale in the x, y, and z directions.

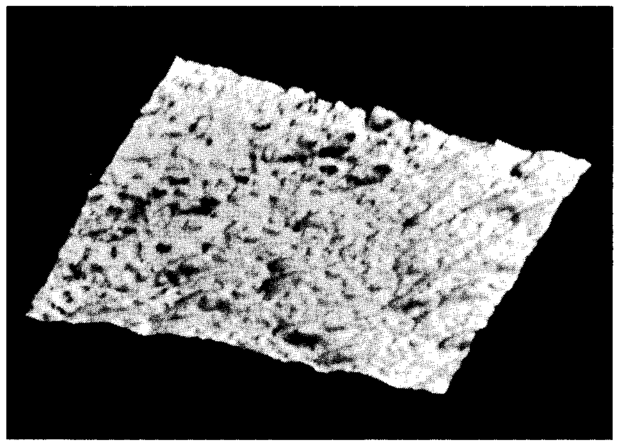

Figure 3

The STM image of Figure 2 seen in an oblique perspective.

Summary

We have described and discussed a computer system for the control of scanning tunneling microscopes, and the acquisition and real-time display of the data thus acquired. This system is based upon the IBM Personal Computer Model AT or XT, using the standard IBM Data Acquisition and Control Adapter card and the Professional Graphics Controller card. The software is organized in a way that will allow the future replacement of these cards by others more efficient. The intent of this system is to provide STM users with a readily available and convenient tool for data collection and observation.

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