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Digital scanning probe microscope controller for molecular manipulation applications

M. J. Humphry, R. Chettle, P. J. Moriarty, M. D. Upward, and P. H. Beton[a)]
School of Physics and Astronomy, University of Nottingham, University Park, Nottingham NG7 2RD, United Kingdom

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A versatile digital controller for scanning probe microscopy capable of data acquisition during molecular manipulation has been constructed. A commercially available digital signal processor (DSP) board connected to a Pentium PC and custom-built high voltage amplifiers were used to control a commercial ultrahigh vacuum scanning tunneling microscope and to perform molecular manipulations. Use of the DSP system to produce all analog outputs resulted in an extremely flexible system with complete control of the probe tip. © *2000 American Institute of Physics.* [S0034-6748(00)00604-3]

I. INTRODUCTION

Control of scanning probe microscopes (SPM) using digital systems is becoming increasingly common due to their greater flexibility as compared with analog systems. Digital signal processors (DSPs) are designed for high data rate real-time processing of analog signals, which makes them ideal for digital SPM control. Several recent articles[1–4] have described SPM controllers based on DSPs utilizing various different digital feedback algorithms and system architectures. In this article, we present a versatile DSP system that utilizes multichannel digital to analog converters (DACs) and analog scan window rotation to allow complete control over the SPM tip. The control algorithm we have chosen is a basic three-term controller (proportional-integral-differential, or PID) which is implemented on the DSP in C code.

A key aspect of our instrumentation is its use for manipulation applications. Controlled movement of individual atoms was first demonstrated by Eigler and Schweizer.[5] In these experiments, which were performed at 4.2 K, xenon atoms were manipulated into ordered patterns on a copper surface. This manipulation technique was subsequently extended to room temperature operation using buckminsterfullerene (C_{60}) on a Si(111) surface.[6] The interaction of C_{60} with the Si(111)-7×7 surface inhibited diffusion at room temperature but was sufficiently weak to permit scanning tunneling microscope (STM) induced movement of molecules. The interactions between the STM tip and molecules are complex and are not yet fully understood, as the use of commercial electronics[7] has limited the range of data that may be acquired during the manipulation process. The system described later has been designed to investigate this interaction by enabling acquisition and systematic variation of tunnel current and tip position during room temperature molecular manipulations.

[a)]Electronic mail: peter.beton@nottingham.ac.uk

II. HARDWARE

Our experimental setup consists of a commercially available room temperature ultrahigh vacuum (UHV) STM[7] controlled by the DSP system described later. At the heart of our control system is a Texas Instruments TMS320C32—a 32-bit floating point processor interfaced to a Pentium PC using a board provided commercially by Blue Wave Systems.[8] The board contains an area of fast access zero wait state static random access memory (SRAM) for DSP program storage, plus an area of shared dual port RAM for data transfer between DSP and PC. Analog inputs and outputs are provided by a plug-in module for the DSP board consisting of two 200 kHz 16-bit analog to digital converters (ADCs) and two 200 kHz 16-bit DACs. A separate board connected to the DSP via the 50-way DSP-link system developed by Loughborough Sound Images (now Blue Wave Systems), provides an additional sixteen 12-bit DACs. The DSP board is housed in an industry standard architecture (ISA) expansion slot on a basic 133 MHz Pentium PC running Windows 95. In addition to the DSP boards, the PC also contains a digital output board for control of some functions of the high voltage (HV) amplifiers described later.

A set of custom-built HV amplifiers provide the signal conditioning required to produce the wave forms that drive the piezoelectric tube in the STM head. The piezoelectric tube has four quadrants, so the outputs from the HV amplifiers must take the form $(Z+X)$, $(Z-X)$, $(Z+Y)$, and $(Z-Y)$. The axes are defined according to the standard convention in which the Z axis is parallel to the STM tip.

Figure 1 shows a block diagram of the system architecture. It can be seen that the amplifier has two inputs for each axis (X, Y, or Z), labeled offset and fine. The offset inputs are amplified by a fixed amount to produce a full-range output of ±150 V. The fine channels have a variable gain determined by digital outputs from the PC. The X and Y offset channels are used to locate the origin of a scan within the full range of the piezoelectric tube. The X and Y fine channels are then used to raster scan the tip to form an image. Both the offset and fine inputs for the X and Y channels are produced by the

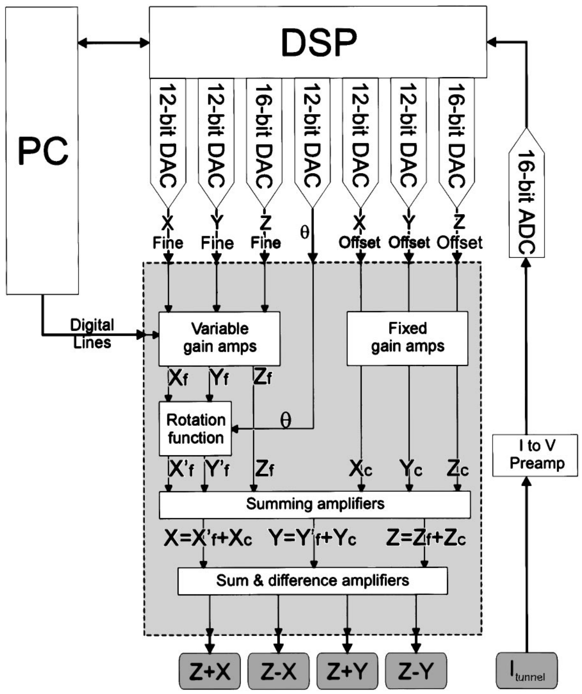

FIG. 1. A schematic of our SPM control system. The shaded rectangle represents the analog HV amplifier unit.

12-bit DACs connected to the DSP. The X and Y fine DAC outputs are ramped over their full range of 12 bits during each scan. The size of the scan window is determined by the gain of the X_{fine} and Y_{fine} channels on the HV amplifier set by digital outputs from the PC. Therefore, the minimum $X-Y$ voltage step is always 1/4096 of the full DAC output range, independent of scan size.

The Z channels are operated in a similar manner to X and Y, with the offset channel used to establish the coarse Z position. The gain on the fine Z channel is also variable to allow the minimum Z voltage increment (limited by digitization) to be decreased for very flat surfaces, or increased for rough ones. The digitization errors in Z must be smaller than those for X and Y due to the greater resolution of a SPM in the Z direction compared to X and Y. The offset and fine inputs for the Z channel are therefore generated by 16-bit rather than 12-bit DACs.

An additional analog output (θ) is used to apply a hardware rotation to the scan window defined by the X and Y fine channels—a very important function that will be discussed in detail in the next section. The coarse and fine channels are then summed and either added or subtracted from Z using sum and difference amplifier circuits to produce the required outputs. All analog inputs to the HV amplifiers are provided by the DSP controlled DACs. This method is somewhat different to other recent DSP based systems that rely on an additional output board in the PC to provide the X and Y inputs.[2–4] Controlling all the inputs to the HV amplifiers from the DSP in this way means that the system is extremely flexible and that tip movement and data acquisition may be readily synchronized. However, this flexibility is at a slight cost of speed. The feedback update rate discussed later is typically 25 μs compared with $\sim$15 μs quoted elsewhere.[1,2]

III. SOFTWARE

All digital control systems require a feedback calculation to be performed at regular intervals to maintain a physical parameter at a given level (for example tunnel current). The algorithm we use is the common PID loop. Under PID control, a term proportional to the difference between the current value of the controlled parameter and its desired value is added to terms proportional to the integral and derivative of the difference. The controller then outputs the result of the sum.

For a digital system, the algorithm can be written as follows:

$$Z_i = PE_i + Z_{i-1} + I(E_i + E_{i-1}) + D(E_i - E_{i-1}), \tag{1}$$

where i is the iteration number, Z_i is the ith output, E_i is the ith value of the difference between measured and required values and P, I, and D are constants.

The DSP software was written in C and was based around the configurable ADC sample timer on the DSP board. This timer generates an interrupt to the DSP every time an ADC sample is available and can be set to frequencies up to 200 kHz. For the purposes of this SPM control application, the timer is set to 40 kHz.

The most important feature of the DSP program is the interrupt service routine (ISR) that responds to the ADC interrupt. A system of control variables has been developed similar to that employed in the Windows 95 operating system. A central control variable is examined every time the ISR is executed. A different function is then called depending on the state of the control variable. Subroutines to perform tasks such as the acquisition of a data point or movement to the next image point may be called as appropriate. This system enables the addition of new functionality to the system without excessive modification.

The ability to rotate a scan window is often useful and is particularly important for manipulation applications. Scan rotation can be produced by a calculation in software that results in a simultaneous variation in X_{fine} and Y_{fine} outputs. For rotation angles that are noninteger multiples of $\pi/2$, implementation of rotation in software results in a decrease in scan size and a stepped structure on the tip trajectory due to digitization. To overcome these problems, an analog rotation function has been implemented in the signal conditioning stages of the fine channels of the HV amplifiers. The rotation combines the X and Y fine inputs according to the following equations using sine-cosine operational amplifiers:

$$\begin{aligned} X'_f &= (X_f \cos\theta - Y_f \sin\theta), \\ Y'_f &= (X_f \sin\theta + Y_f \cos\theta). \end{aligned} \tag{2}$$

The result is a scan window with full 12-bit voltage accuracy where the X axis can be rotated by any given angle, θ, without a change in size of the window or increase in digitization errors. In addition, the STM tip always moves in the same direction during manipulation and it is possible to avoid irregular displacements (see Fig. 2). In practice the orientation of the scan window must thefore be rotated so that the direction for manipulation is aligned with either the X'_f or Y'_f axes.

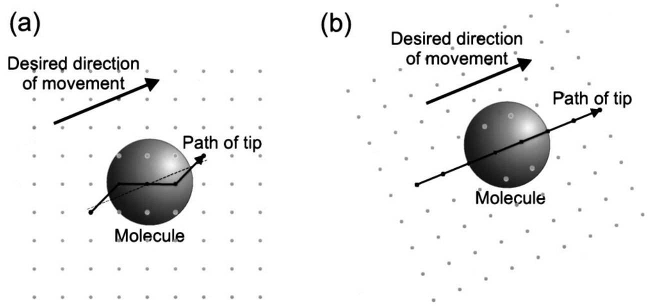

FIG. 2. Comparison of STM tip trajectory during a manipulation procedure with digital and analog scan rotation. (a) Scan rotation performed digitally in software. The small gray dots represent possible tip positions (limited due to digitization of DAC outputs). The tip trajectory forms a stepped structure as an approximation to the desired direction of motion. (b) The array of addressable points is rotated by analog electronics to align the primary axes with the desired direction of manipulation. The tip trajectory forms a continuous line, enabling controlled manipulation experiments to be performed.

User interaction is provided by a front-end written in Visual BASIC that accepts values for parameters such as PID constants and the control variable and passes them to the DSP program via the dual port RAM on the DSF board. Similarly, data from each scan line is returned to the PC via dual port RAM after acquisition. All image processing functions such as plane subtraction, interpolation for zoom purposes, line normalization, and derivative calculations have been implemented in C++ and compiled into a dynamic link library that can be called from Visual BASIC. It was necessary to write these functions in C++ due to the large increase in speed this offered over Visual BASIC.

A set of DSP routines has been written to extend the simple room temperature molecular manipulation experiments of C_{60} performed previously by our research group.[6] The routines allow the STM tip to trace a horizontal or vertical line (defined using Visual BASIC on a previous scan) forwards and backwards a predetermined number of times. Different tunneling parameters can be independently defined for the forward and reverse directions allowing conditions likely to cause motion of a molecule[6] to be set up for one direction only. Values of tunnel current and Z position during each trace may be acquired by the DSP and passed to Visual BASIC to be displayed. Using this data, the position of a molecule can be determined on a forward trace and an attempt to move it can be performed on the reverse trace. A second forward trace can determine whether the molecule has moved. The flexibility of our controller enables systematic variation from trace to trace of the parameters that characterize the response of the control system (e.g., X/Y step size, samples/point etc.) in order to investigate their effect on molecular manipulation.

IV. RESULTS

The control system has been successfully used to acquire images with atomic resolution on two different silicon surfaces, Si(100)-2×1 and Si(111)-7×7 as shown in Fig. 3. The images are virtually indistinguishable from those obtained

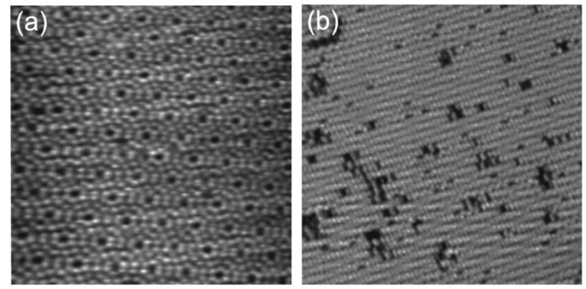

FIG. 3. Atomic resolution images of two different silicon surfaces acquired using the instrumentation described earlier. (a) 200×200 Å image of Si(111)-7×7 (sample bias 3 V, tunnel current 0.2 nA). (b) 230×230 Å image of Si(100)-2×1 (sample bias −2.5 V, tunnel current 0.2 nA).

using our commercial controller with the same UHV STM head. Individual Si dimers can readily be resolved on the Si(100)-2×1 surface.

The controller has also been used to perform molecular manipulation experiments on C_{60} using the manipulation procedures described in the previous section. Figures 4(a)–4(b) show images before and after an attempt to manipulate a C_{60} molecule along a trough between dimer rows.[9] The molecule in the center of the image has been displaced through 15.4 Å (four unit cells) by the manipulation procedure applied between scans.

The trajectory of the tip during manipulation is indicated by the horizontal line in Fig. 4. Figure 5 shows the Z position and tunnel current during the application of the manipulation procedure (previously unavailable with our commercial system). The traces with open symbols were acquired with an applied sample voltage of −3.5 V and tunnel current −0.1 nA (parameters which are routinely used for imaging) with the tip moving from right to left (as indicated in the inset). The traces with filled symbols were acquired with voltage 1 V and tunnel current 1 nA with the tip moving from left to right. The line scans were performed in the sequence 1a, 1b, 2a, 2b, 3a. The 7 Å protrusion on the (right to left) Z position ''a'' traces corresponds to the C_{60} molecule, and the smaller periodic bumps are Si dimer pairs. These features are not present in the forward Z position line scans, where the tunnel gap impedance was reduced from 35 to 1 GΩ to facilitate manipulation.[9] Note that the reduction in tunnel gap impedance results in a reduction of the tip-sample separation. Following this repositioning the rate of change of the logarithm

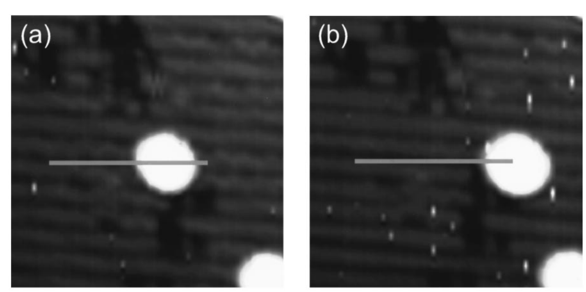

FIG. 4. Controlled manipulation of a C_{60} molecule on Si(100)-2×1. (a) Before manipulation is performed—line shows trajectory tip follows during manipulation procedure. (b) After manipulation—molecule has moved along the trough between dimer rows by four unit cells (15.4 Å). Images are 80 Å×80 Å in size.

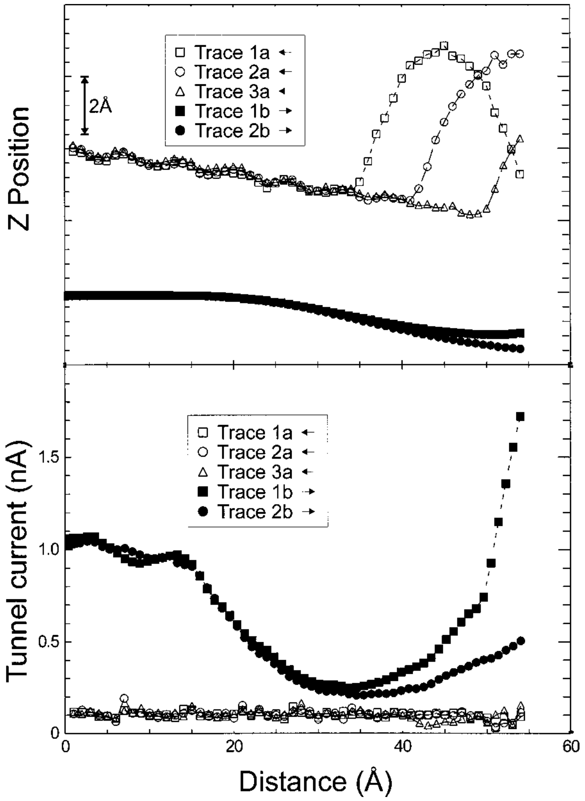

FIG. 5. Plots of data acquired during manipulation procedure in Fig. 4: upper—Z position data; lower—tunnel current.

of current with tip-sample separation will also change, so that the overall feedback parameters are modified although the numerical value of the constants specified in Eq. (1) are unchanged.[10] The lack of features on the forward Z position traces suggests that the STM tip does not respond fully to the presence of the C_{60} molecule indicating that the interaction between tip and molecule that leads to displacement is repulsive. The corresponding tunnel current traces show minimal variation during each a trace as the tip follows the topography. However, there are large variations in ''b'' tunnel-current traces and a marked increase in tunnel current at the position of the C_{60} molecule indicating that for these parameters the feedback response is not effective. An important observation from the acquired data is that the C_{60} molecule does not move through its total displacement in one step. These preliminary results show that the molecule moves in steps of two unit cells.

In summary, we have constructed a versatile DSP-based scanning probe controller with molecular manipulation capabilities and demonstrated its operation by manipulation of C_{60} in UHV on a Si(100) 2×1 surface.

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