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Research Report

EVALUATION OF THE STM MEASUREMENTS OF THE Si(111) SURFACE

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Typed by: A. Schönholzer on IBM MC82C

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ABSTRACT: The distortive response of a conventional X-Y recorder can be described by a convolution of the input signal with the complex susceptibility of a damped harmonic oscillator. The characteristic parameters of the damped harmonic oscillator were obtained by recording rectangular input signals at a given speed and sinusoidal signals at a given frequency. The processed STM image of a Si(7×7) surface satisfies the trigonal symmetry.

February 9, 1984

Introduction

The originally recorded STM(7×7) data [Fig. 1, G. Binnig *et al.* (1983)] were split into three sets, to avoid bifurcation and crossing points, (Figs. 2-4), and scanned with a resolution of 508 pel/inch in the x-, and 500 pel/inch in the y-directions.

The traces of the extracted lines are shown in Fig. 5. This plot can be compared with the original data (Fig. 1).

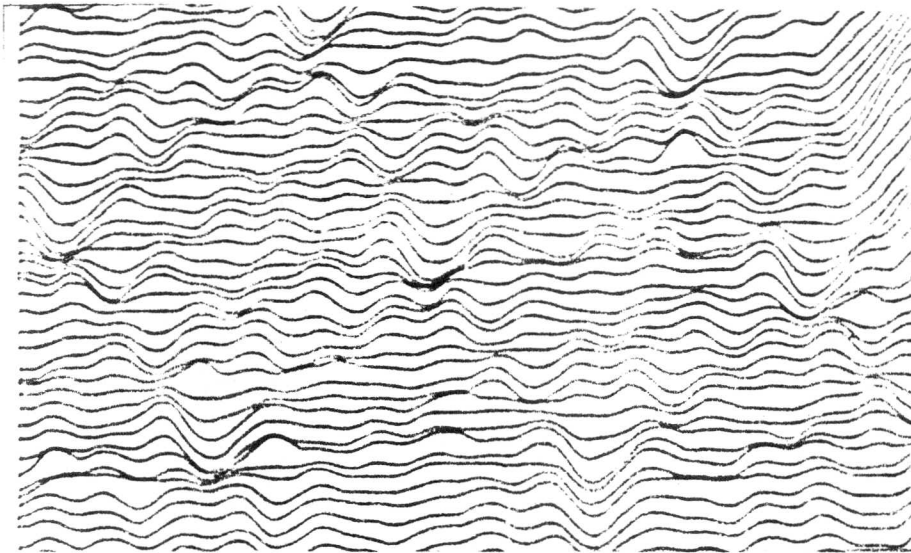


Fig. 1: Si(111) surface as output on XY plotter of the STM (October 18, 1982).

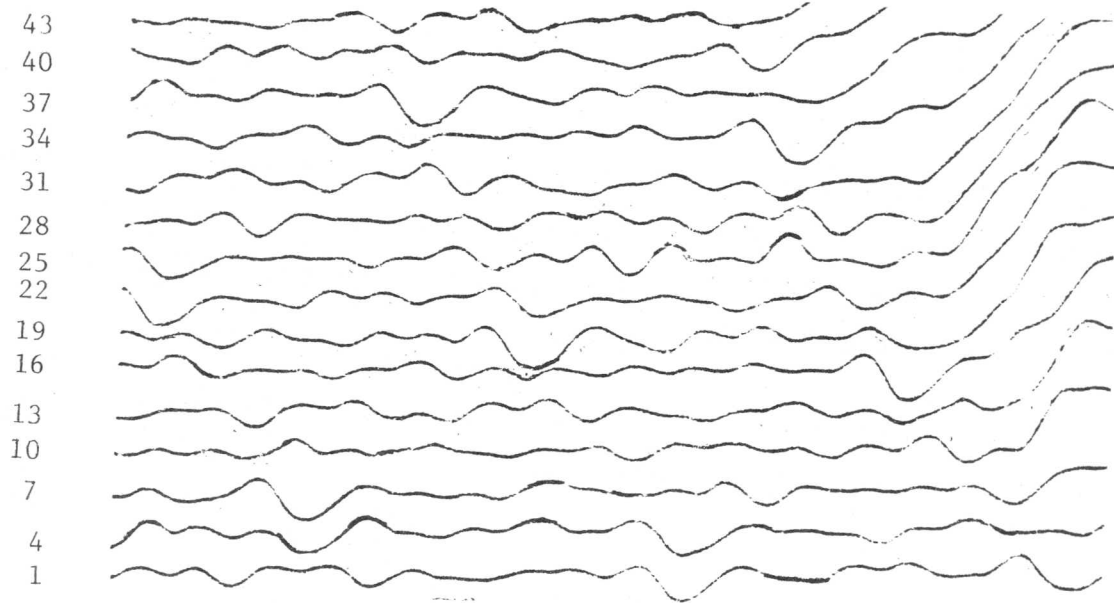


Fig. 2: First set of curves extracted from Fig. 1.

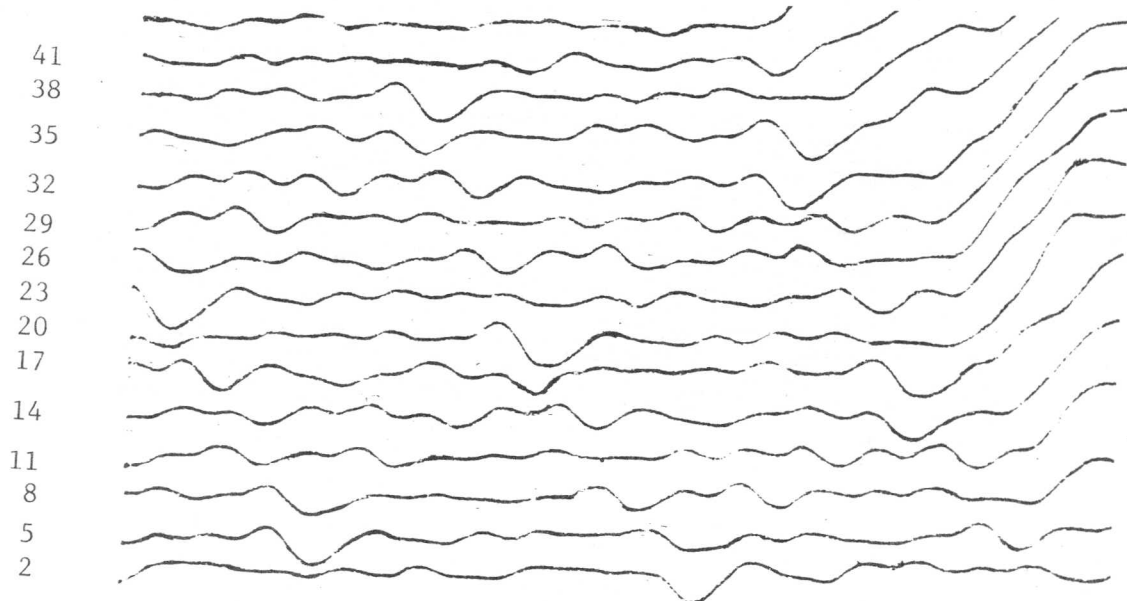


Fig. 3: Second set of curves extracted from Fig. 1.

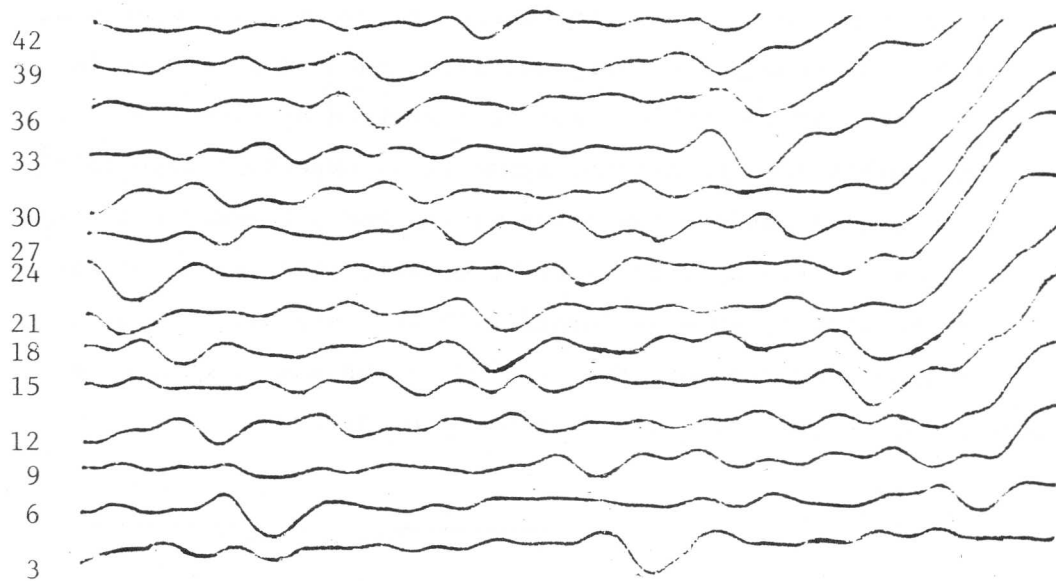


Fig. 4: Third set of curves extracted from Fig. 1.

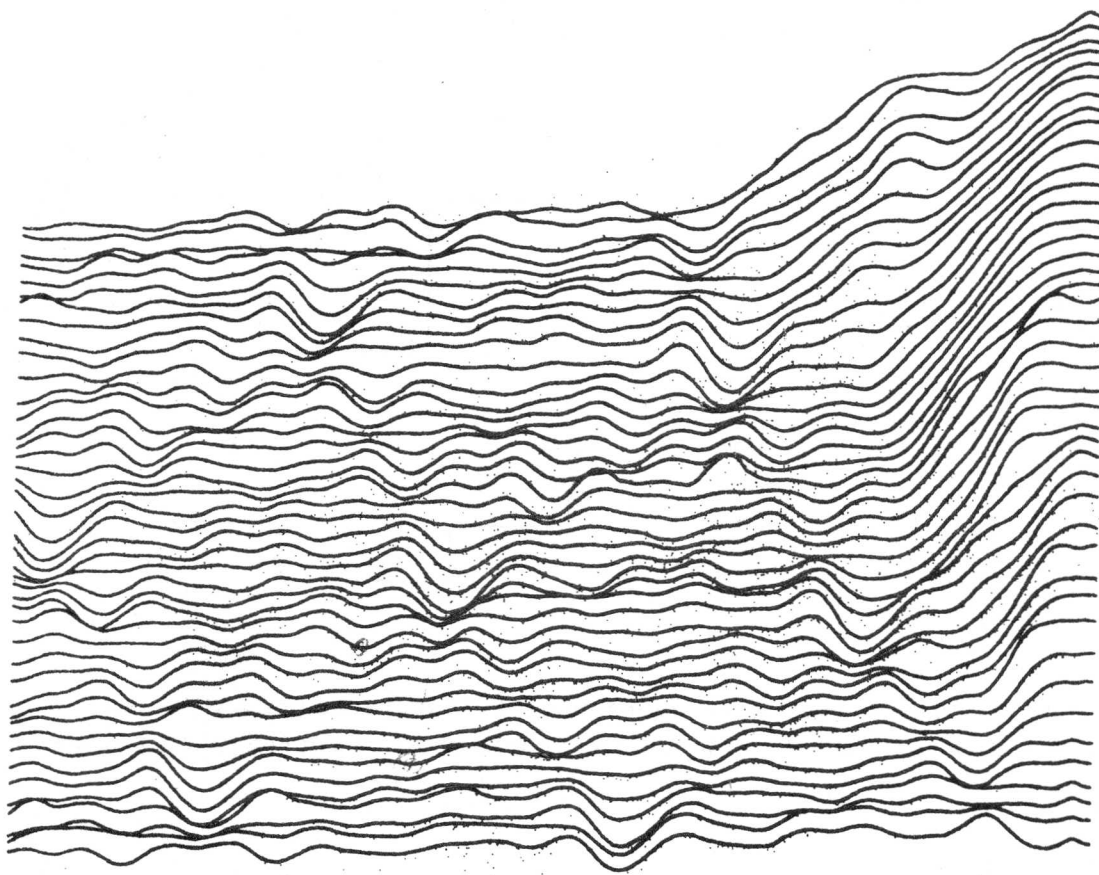


Fig. 5: Output of digitized data.

The next problem to be solved was compensation for mechanical overshoot of the plotter which recorded the original data. Such an overshoot is indicated by the fact that the silicon surface reported by Binnig *et al.* (1983) did not exhibit 120° rotational symmetry as expected; especially the "connecting" minima between two major minima had differences in depth being related to the scanning direction. To measure this overshoot, some experiments on the plotter were performed with test signals showing a resonance frequency close to some frequencies in the data (Figs. 6 and 7). On the other hand, no nonlinear distortions were observed.

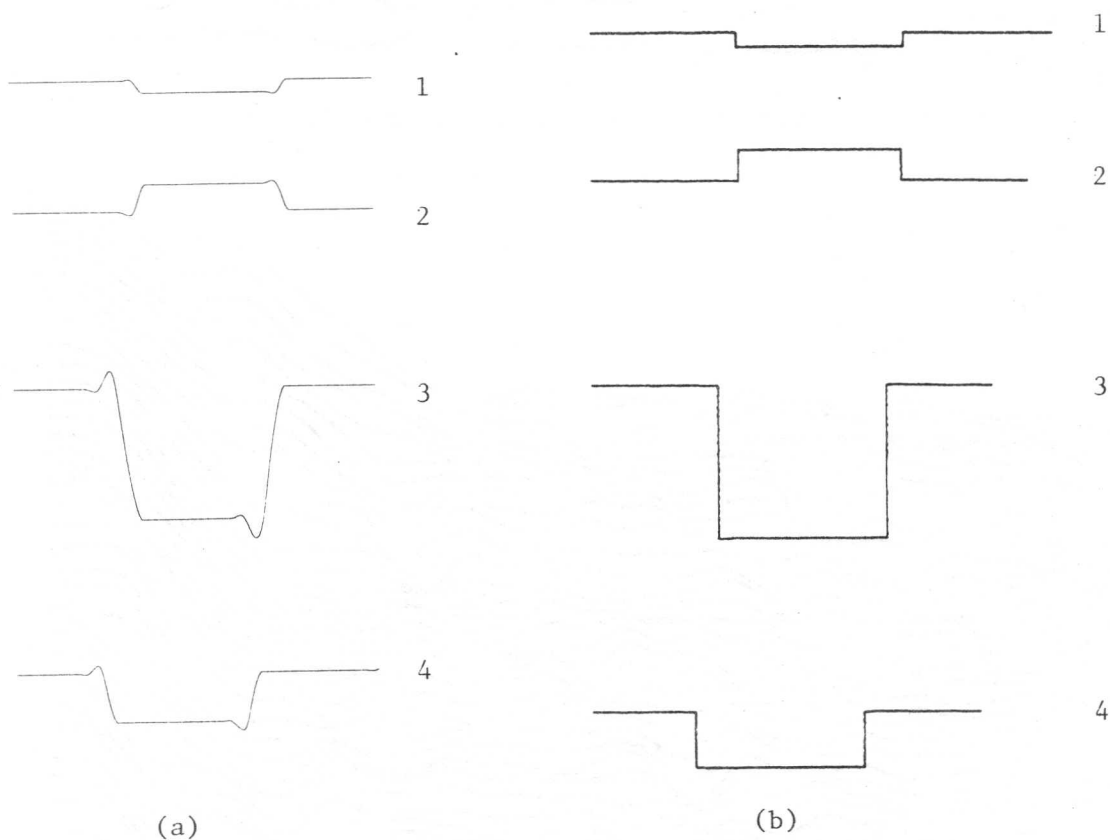


Fig. 6(a): Plotter output with overshoot of fast rectangular pulses.
 (b): Plotter output without overshoot of slow rectangular pulses.

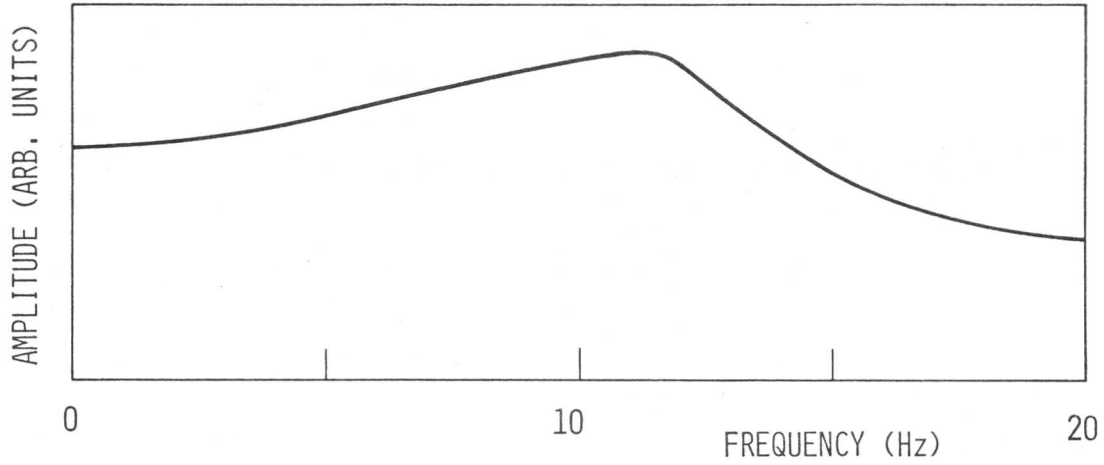


Fig. 7: Resonance curve of plotter of input signal with constant amplitude and increasing frequency.

In order to restore the data, the following distortion model is proposed:

Distortion Model for Overshoot Phenomena

According to the mechanical and electronic design of the plotter, the relaxation between input signal $y(t)$ and recorded signal $x(t)$ can be described by the equation of motion

$$m\ddot{x} + c\dot{x} + k(x-y) = 0, \quad (1)$$

where m is a characteristic mass of the recorder drive, and c and k correspond to the damping and restoring forces given by the electro-mechanical design of the recorder.

By Fourier transforming this equation, using

$$x(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} X(\omega) e^{-i\omega t} d\omega, \quad (2)$$

$$y(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} Y(\omega) e^{-i\omega t} d\omega, \quad (3)$$

and assuming that $c = m\gamma$, and $k = m\omega_0^2$ we then get

$$X(\omega) = \frac{\omega_0^2 Y(\omega)}{\omega_0^2 - \omega^2 - i\gamma\omega}, \quad (4)$$

with

$$R(\omega) = \frac{\omega_0^2}{\omega_0^2 - \omega^2 - i\gamma\omega}, \quad (5)$$

and

$$X(\omega) = R(\omega)Y(\omega). \quad (6)$$

$1/\omega_0^2 R(\omega)$ is the complex susceptibility of a damped harmonic oscillator, becoming overdamped for $\gamma = \sqrt{2}\omega_0$.

The product of $R(\omega)Y(\omega)$ in Eq. (6) means that the recorded signal $x(t)$ is the convolution of the input signal $y(t)$ and the oscillator function $r(t)$ given by the design of the xy recorder.

The distortion process now performs the inverse transformation of (6) on the recorded output signal in order to arrive at the undistorted input signal

$$Y(\omega) = \frac{X(\omega)}{R(\omega)} = \frac{1}{\omega_0^2} ((\omega_0^2 - \omega^2) - i\gamma\omega) \cdot X(\omega). \quad (7)$$

In practice, where finite Fourier transforms and discrete data samples are used, the filter $1/R(\omega)$ must be multiplied with some suitable low-pass filter $L(\omega)$ to prevent magnification of noise by the deconvolution process. The low-pass filter used for the restoration of the silicon surface was

$$L(\omega) = \frac{1}{1 + \left(\frac{\omega}{\omega_c}\right)^{2n}}, \quad (8)$$

where n was chosen equal to 2, because $1/R(\omega)$ grows with the square of ω .

Restoration of the Si(111) surface

The 43 lines of the original recording of the silicon surface were converted into "heights" according to the following procedure:

First, each line was convolved with $L(v)/R(v)$, where

$$v = \frac{\omega}{2\pi}, \quad v_0 = \frac{\omega_0}{2\pi} = \frac{1}{190} \text{ peV}^{-1} = 1.053 \text{ cm}^{-1},$$

$$\gamma = 0.022 \text{ and } v_c = \frac{\omega_c}{2\pi} = 1.73 \text{ cm}^{-1}.$$

These values were chosen because they enhanced the 120° rotational symmetry of the surface, and because they agreed well with values derived from the test plots (Figs. 6 and 7).

Next, the average slope of each line was calculated, and a mean slope of all 43 lines was used to determine a straight line with minimal square error for each line recorded. The differences between each line recorded and its corresponding straight line were taken as "heights" using the conversion factor

$$1 \text{ cm} \approx 5.8 \text{ \AA}.$$

The distance of each scan from the next was assumed to be constant. It was determined using the *a priori* assumption that the deep minima are arranged in a grid of equilateral triangles. A nonlinear drift from one scan to the next owing to thermic changes during recording, was modeled as a parabola, and determined using the same assumption. This accounts for the round edges on both sides of the image of the restored silicon surface (Fig. 8).

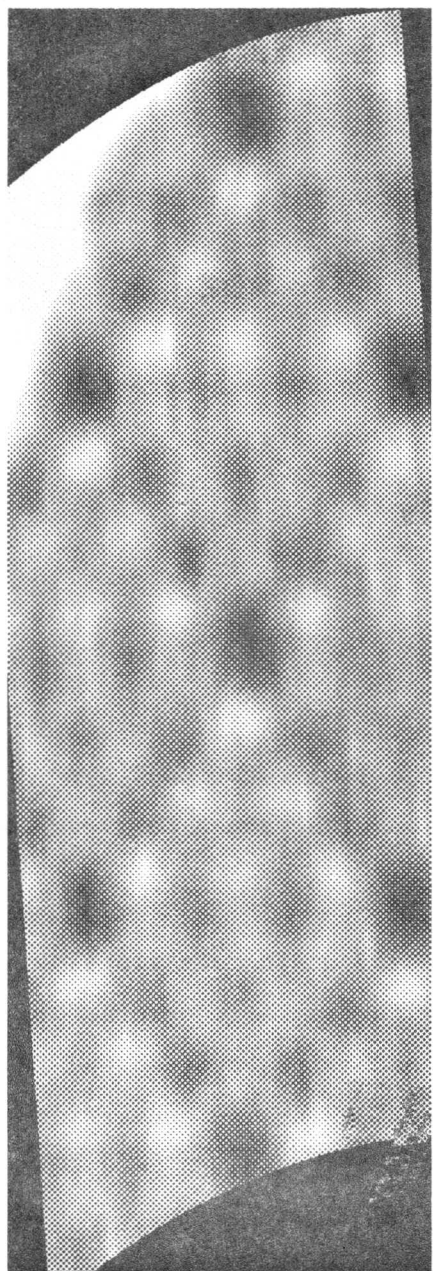


Fig. 8: Top-view of overshoot-corrected Si-111 surface with depth proportional to darkness.

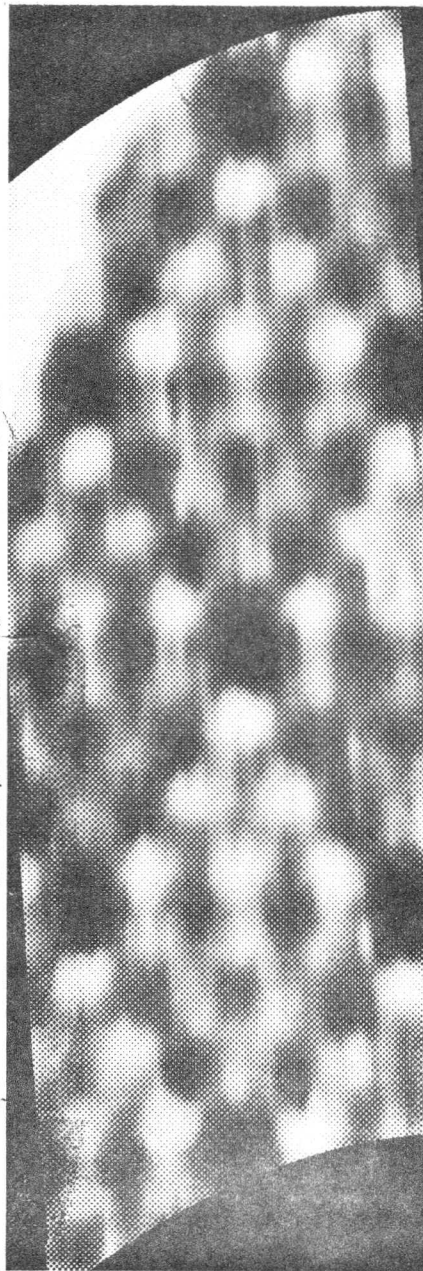


Fig. 9: Same as Fig. 8 but with contrasts enhanced.

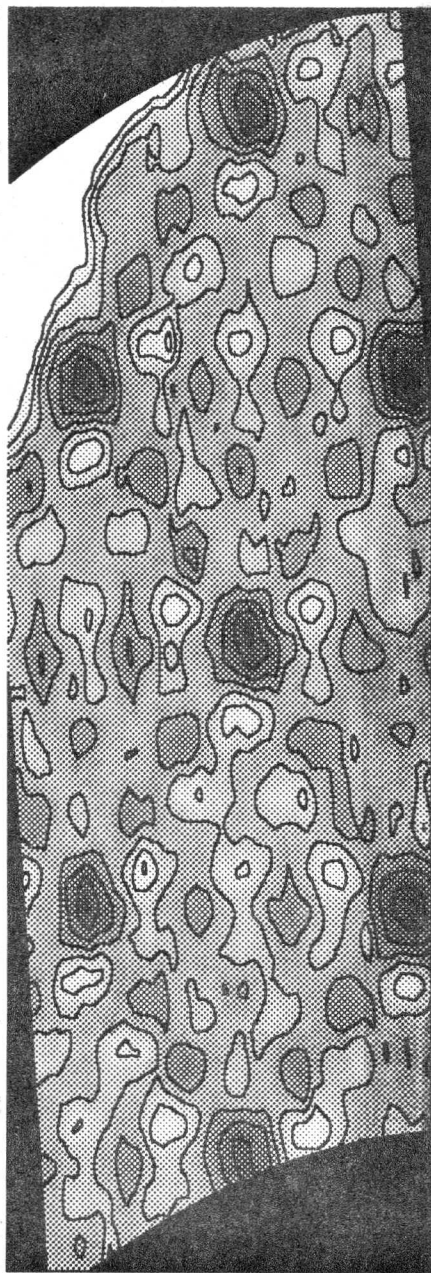


Fig. 10: Same as Fig. 8 but with contour lines at 0.5 Å intervals.



Fig. 11: Same as Fig. 8 but with contour lines at 0.2 Å intervals.

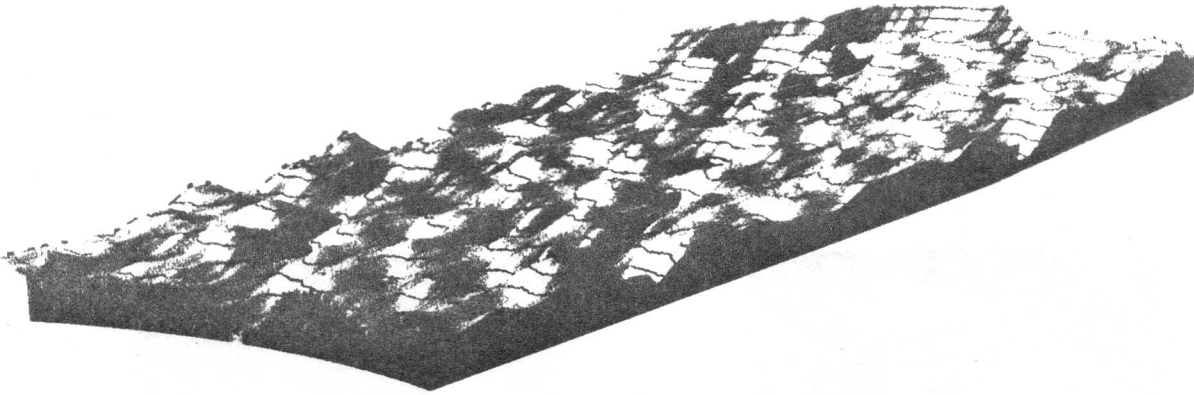


Fig. 12: Three-dimensional view of overshoot-corrected Si-111 surface.

This surface was printed in several ways in order to exhibit its structure. In Fig. 8, the grey levels are proportional to depth, where the difference between complete white and total dark is 3.2 \AA . Figure 9 is the same as Fig. 8 except that the grey levels were chosen for maximal contrast and do not represent the heights faithfully.

Figures 10 and 11 show the same as Fig. 8 with z-contours at 0.5 \AA and 0.2 \AA distances, respectively. Finally, Fig. 12 gives a three-dimensional overview of the surface investigated.

Conclusions

The method described using a damped harmonic oscillator model to explain overshoot phenomena to restore the original data before distortion by a linear system black box is quite uncomplicated and useful. It involves estimation of two parameters (γ and ω_0) which cannot be derived from the distorted data direct but can be obtained by recording well-defined input signals. As overshoot phenomena can occur in many portions of the measuring process, the method given here is not limited to the compensation of overshoot in x-y plotters.

References

- ¹G. Binnig, H. Rohrer, Ch. Gerber and E. Weibel, Phys. Rev. Lett. 50, 120 (1983).