Amplitude of the atomic corrugation of a cleaved bismuth surface measured with a scanning tunneling microscope

A. M. Troyanovskiĭ

Institute of High Pressure Physics, Russian Academy of Sciences, 142092 Troitsk, Moscow Region, Russia

V. S. Édel'man

P. L. Kapitsa Institute of Physics Problems, Russian Academy of Sciences, 117334 Moscow, Russia

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The amplitude of the atomic corrugation, A, and the change in the gap between the sample and the scanning tip, δZ, have been measured as a function of the voltage across the tunneling gap at a fixed current, i.e., as a function of the resistance of the tunneling gap, R_T, by scanning tunneling microscopy. The results show that A increases slightly, from 0.5 ± 0.1 to 0.7 ± 0.1 Å, as R_T is raised from 40 to ~200 MΩ. It then falls off to ~0.5 Å at $R_T\simeq1$ GΩ, provided that the shape of the scanning tip does not change during the measurements. The criterion for a constant tip shape was that the $\delta Z(R_T)$ dependence be the same as that expected for vacuum tunneling at a work function of 4.4 eV. © *1994 American Institute of Physics.*

The observation of metal surfaces at an atomic resolution by scanning tunneling microscopy (STM) has been reported in several papers (see, for example, Refs. 1–3 and some reviews[4,5]). However, we do not yet have a comprehensive picture of the mechanism by which the image is formed. In the first place, it is not clear just why the observed amplitude of the atomic corrugation, A, is often one or two orders of magnitude greater than that expected from the theory of Ref. 5. The amplitude was renormalized in Refs. 6 and 7 for the interaction of the surface atoms with atoms at the end of the scanning tip, but those results are rather difficult to compare with experiment. The reason is that the electron density was calculated as a function of the sample–tip distance in those papers, and this distance is not measured directly in experiments and is thus known only poorly. It was mentioned in Ref. 3 that a large amplitude of the atomic corrugation on the [001] surface of lead is difficult to explain by the approaches of Refs. 6 and 7.

We believe that one important reason for the unsatisfactory state of affairs here is that the experimental information is incomplete. In the papers of which we are aware, there has been no systematic study of how the parameters of the STM image depend on such a factor as the resistance of the tunneling gap, R_T, with simultaneous measurements of the effective work function W, found from the change (δZ) in the sample–tip distance upon a change in R_T. It has been found[1] in a study of aluminum that the dependence $A(R_T)$ is approximately a $1/\sqrt{R_T}$ dependence, with A falling off from 0.8 to 0.15 Å as R_T is increased from 1.25 to 20 MΩ. A similar correlation has been seen[3] for lead.

However, in those papers and also in many others it has been mentioned that there is always an unknown factor: the structure of the microscope tip. This structure may change abruptly and irreversibly in the course of experiments. Furthermore, as we will show below, there is the possibility of reversible changes in the end of the tip upon a change in the sample–tip distance, so caution should generally be exercised in analyzing results.

We accordingly carried out an STM study of the surface formed by cleaving a Bi sample in the basal plane for various values of R_T. The method for preparing the atomically clean surface through cleavage of a Bi crystal is described in Refs. 8 and 9, as is the design of the microscope. In this letter we will focus on only the experimental procedure. To obtain a set of STM images for various values of R_T, we took an approach like that proposed in Ref. 10: While scanning a frame at a constant tunneling current, we changed the voltage between the tip and the sample, U_{t-s}, upon the completion of a line (the coordinate X). The same line was then scanned again. We were able to set several values of the voltage (in practice, up to eight), instead of the two in Ref. 10. Only after scanning the same line at all these voltages did we return to the original value of U_{t-s} and move on to a new line (making a step along Y). In most cases we repeated the original value of the voltage at the middle of the cycle, so that we could obtain two images at the same value of U_{t-s}. By comparing them we could draw conclusions about the reproducibility of the pattern, and we could estimate the drift of the microscope. Repeated measurements of the current–voltage characteristics of the tunneling gap in the course of these experiments revealed that these characteristics are linear over the interval $U_{t-s} \approx \pm 0.1$ V. Above 0.2 V, they acquire a significant nonlinearity. Accordingly, a change in U_{t-s} at a fixed current is equivalent to a change in R_T in the voltage interval just specified.

When the scanning of a frame was completed, the computer memory contained several images like that in Fig. 1a. By subtracting one file from another we were able to find the tip displacement δZ along the normal to the surface upon a change in U_{t-s}, on the average over the frame. Shown at the bottom of Fig. 2 are values of $\delta Z[\log(U_{t-s})]$ for a series of measurements carried out over 1 h. The procedure described above yielded $\delta Z < 0.05$ Å at equal values of the voltage.

It can be seen from Fig. 2 that there are two types of $\delta Z[\log(U_{t-s})]$ curves. For some of the cycles in terms of the voltage (points 4, 5, and 8 in Fig. 2), all the points conform to a straight line, within the measurement error. The slope of this line corresponds to the functional dependence

$$\ln[R_T(Z)] = \text{const} + (2Z/\hbar)(2mW)^{1/2}, \tag{1}$$

where m is the mass of an electron, and the work function $W = 4.4$ eV—the handbook value of the work function for Bi—is essentially the same as $W = 4.5$ eV for tungsten, from which the tip was made. For other cycles, the behavior was different: As U_{t-s} was raised over the interval 12–15 mV, the position of the tip changed rapidly, but with a further change in the voltage all points conformed to a new straight line, whose slope was the same as that of the first one. In a transitional voltage region (points 7 in Fig. 2) we observed a special case: At voltages near 12–15 mV the noise level on the STM images increased sharply. The noise became a random telegraph signal; the time spent in the states corresponding to the lower and upper straight lines was on the order of several tens of milliseconds.

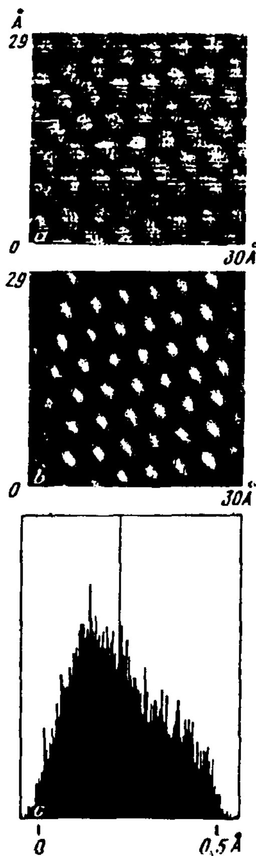

FIG. 1. a—Original STM image of a cleaved Bi surface; b—image after Fourier filtering (the change in level from dark to light is 0.5 Å); c—histogram of the levels for image b. The tunneling current was 0.05 pA, the sample–tip voltage U_{t-s} was 80 mV, and the number of points was 128×128. Image a is one of six images recorded during row-by-row scanning with various values of U_{t-s}. They correspond to points 4 in Fig. 2. The total scanning time was 95 s.

The observed behavior can be explained at a qualitative level by assuming that the end of the tip initially has the shape shown schematically in Fig. 2a. As a result of the capture of an extra atom (of bismuth, tungsten, or the residual gas) at the end of the tip, the shape may become that in Fig. 2b or 2c. However, if the binding energies of the two states are approximately the same, this extra atom can switch between these states because of thermal vibrations. At large distances, this effect leads to an increase in the noise (as is observed at $U_{t-s}>0.1$ V). Later, as Z decreases because of van der Waals attraction, the position in Fig. 2b becomes favored from the energy standpoint. When a repulsion becomes predominant, however, the atom jumps to the position in Fig. 2c. The feedback of the microscope changes the position of the tip abruptly in order to reach the previous value of the tunneling current.

This is of course not the only possible model. However, there can be no doubt that the complicated $\delta Z(U_{t-s})$ dependence indicates a change in the structure of the tip. On the other hand, if $\delta Z(U_{t-s})$ follows Eq. (1), then we have a guarantee that (first) the shape of the tip remains constant and (second) a regime of vacuum tunneling is being realized. It is thus legitimate to analyze the behavior of the corrugation amplitude A as a function of the resistance of the tunneling gap only when the latter condition holds.

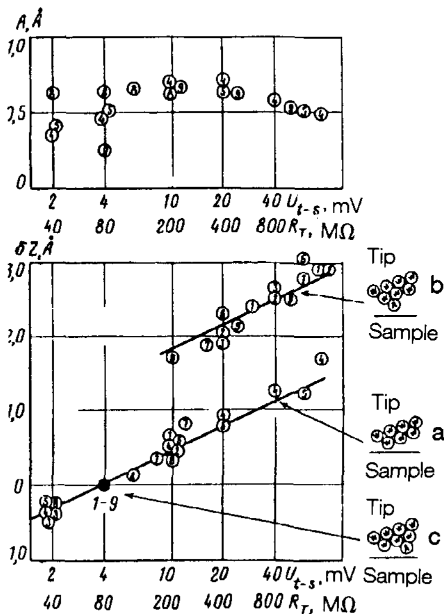

FIG. 2. The amplitude of the atomic corrugation, A (top), and the displacement of the microscope tip, δZ (bottom), versus the voltage U_{t-s} (or versus the resistance of the tunneling gap, R). The numbers specify the successive cycles in terms of U_{t-s}, carried out over 1 h. The displacement δZ was reckoned from the value at $U_{t-s}=4$ mV. Shown at the right is a hypothetical shape of the end of a tungsten tip (a) and the change in this shape upon the capture of one adatom, which can be in either of two states, which are approximately equal in energy (b and c).

To eliminate the effect of noise and drift on the results of the $A(U_{t-s})$ measurements, we took 2D Fourier transforms of the data in each file. The spectrum was left with only the components near the three most intense components, corresponding to the hexagonal lattice of the Bi basal plane. We then took inverse Fourier transforms (Fig. 1b) and calculated a histogram of the levels (Fig. 1c). We took the corrugation amplitude to be the width of the histogram at the 10% level; i.e., we discarded the excursions on the large and small sides. The validity of this procedure is confirmed by the agreement of the results for images recorded under identical conditions.

The $A(U_{t-s})$ dependence is shown at the top in Fig. 2. It turns out to be nonmonotonic: A goes through a maximum near those values of U_{t-s} at which the "switching" of the shape of the tip is observed. If the switching model proposed here is correct, then this maximum apparently means that a force interaction is affecting the atomic corrugation, since, according to Ref. 7, the renormalization due to the force under action changes sign upon a change in the sign of the force.

It can be seen from Fig. 2 that with an increase in the tip–sample distance, the corrugation amplitude falls off by a factor of only 1.5 as R_T increases by more than an order of magnitude. Since the value of R_T is a measure of the overlap of the wave functions of the atoms of the surface and the tip, it seems to us that the weak $A(R_T)$ dependence is evidence that there is no renormalization of the amplitude due to this overlap in the range of R_T values studied. We might add that a switching of the tip may lead to a sharp change in the apparent corrugation. For system of points 9, for example, the corrugation amplitude triples as the voltage is raised from 4 to 10 mV, at the same time as the transition to the upper branch of the $\delta Z(U_{t-s})$ dependence.

In summary, we have established that, at a fixed shape of the microscope tip, the

atomic corrugation of a Bi surface depends only weakly on the resistance of the tunneling gap over the range measured. The values which we found can thus be compared with calculations for a free surface, if and when such calculations are carried out.

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