Atomic-resolution STM image of a Pb (001) surface

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Atomically smooth terraces with dimensions of a few hundred angstroms have been observed on a lead (001) surface by scanning tunneling microscopy. The terraces are separated by steps with a height equal to the interplanar distance. An atomic picture of the surface, with an atomic-corrugation amplitude ranging up to 1.4 Å, has been obtained.

The mechanism by which the atomic-resolution image is formed in a scanning tunneling microscope (STM; we will use the same abbreviation for scanning tunneling microscopy) has been studied theoretically in many places [see the reviews (Refs. 1 and 2)]. In semiconductors, the electrons participating in the tunneling are largely localized at lattice ions, so the constant-density surfaces of the electrons exhibit a significant corrugation. Correspondingly, the variations δz in the position along the z axis, which terminates in one atom of the STM tip during scanning of the surface which traces out this corrugation, amounts to something on the order of an angstrom. The situation is different in metals, in which the conduction electrons are not localized, and the amplitude δz is expected to be small at unreconstructed faces.[1] Nevertheless, an atomic surface structure with $\delta z \sim 0.2$–0.5 Å has been reliably observed on several metals: Au, Ag, and Ga (Refs. 3–5, respectively). In addition, δz reaches 1 Å in the case of aluminum, while for graphite it may even exceed the interplanar distance, depending on the experimental conditions.[7] Efforts to explain this anomalous behavior have invoked ideas based on a strong interaction of the tip with the surface atoms. For graphite, with its low stiffness, one might expect an intensification of the effect due to the deformation caused by the tip.[7] In contrast, the explanation of the large amplitude of the effect in the case of aluminum on the basis that easily deformed microparticles adhering to the end of the tip are responsible for the image seems contrived.[6] In this situation, we believe that the results we are reporting in the present letter, on the observation of atomic-resolution images of a lead surface, are of interest.

The measurements were carried out on lead single crystals with dimensions of $4 \times 2 \times 1$ mm cut by an arc method from large planar crystals grown by directed crystallization from the melt in a dismountable, optically polished quartz mold from a starting material with a purity on the order of $10^{-4}\%$. These crystals had been used previously in a study of cyclotron resonance;[8] the observation of this resonance was evidence of the high quality of these crystals. We studied a surface of the crystal which had not been subjected to arc processing. Before it was placed in the STM, the sample was treated in a polishing solution of $H_2CO_3 + 20\%\ H_2O_2$ in order to remove the oxide film, a few microns thick, which formed during storage. In the STM[9] the crystal was in a sample holder which could be heated *in situ* to the melting point of lead. The

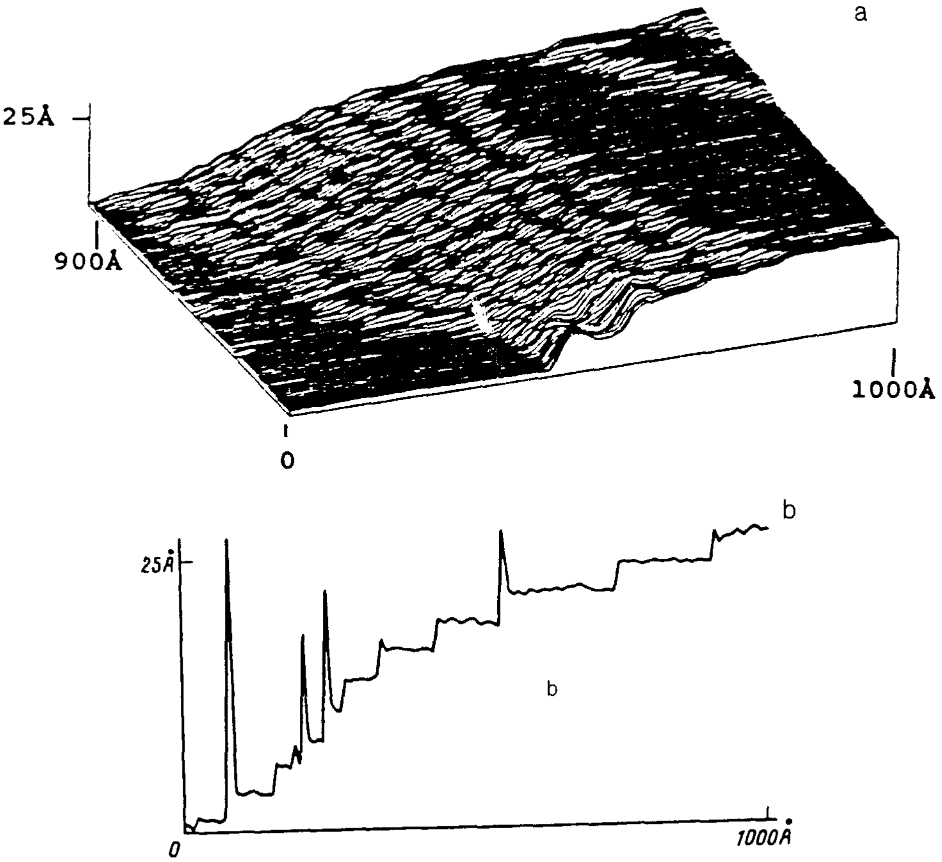

FIG. 1. a: Topogram of part of a lead (001) surface, smoothed to reduce noise. b: Section of this topogram (not processed mathematically) along the most remote line. Steps with a height equal to the interplanar distance in lead, 2.48 Å, can be seen. The tip-sample voltage was 7 mV, and the current 0.13 nA.

measurements were carried out in a vacuum up to 10^{-9} Torr. An atomically clean surface was achieved by bombarding the lead for several hours with 4-keV Ar^+ ions, which were incident on the surface at an angle of 10–20°. The ion current density was on the order of 0.1 $\mu A/mm^2$. The sample was simultaneously heated to 250–300 °C to anneal out defects created during the ion bombardment. After the sample was cooled to room temperature, STM images of various parts of its surface were recorded.

After this surface processing, we observed images of the surface made up of distinct, atomically smooth terraces with sizes ranging from a few tens of angstroms to a few hundred angstroms (Fig. 1). We used the height of the steps between the terraces, which is equal to the interplanar distance in lead, 2.48 Å, to calibrate our STM along the z axis. The signal becomes unstable at the boundary of a terrace: There are spikes in the current and, correspondingly, in the position of the tip, as is clear

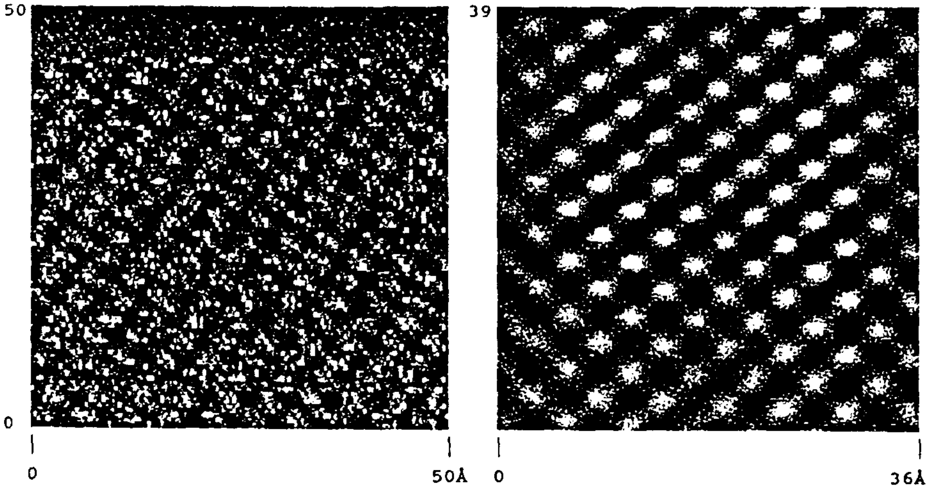

FIG. 2. STM images giving an atomic picture of two regions on a lead (001) surface. a: Experimental image, before noise is filtered out. At the top of this frame one can see the fading of the atomic pattern at the transition from one scanning line to another. The angular distortion is due to drift during the measurements. b: Image of a different region. The noise has been reduced by Fourier processing. The drop from a bright region to a dark region is (a) 2Å or (b) 1Å. The time taken to record a frame is (a) 200 s or (b) 44s. The tip-sample voltage is (a) 7 or (b) 11 mV. The current is (a) 0.13 or (b) 0.1 nA.

from Fig. 1b. Because of this instability, the terrace boundaries look slightly blurred. Although the reason for this effect is not clear at this point, we can rule out a trapping of atoms on the tip, since the levels of the terraces remain the same in the direction perpendicular to the scanning line, and the images are fairly reproducible when the direction of the line scanning and the frame scanning are changed.

Within the individual terraces, the typical noise level is ~0.1 Å. In many cases, a periodic structure corresponding to the symmetry of the (001) plane can be seen clearly on the STM images (Fig. 2). The amplitude of the atomic corrugation, δz, varies from experiment to experiment. There is a correlation between this amplitude and the experimental conditions: As the resistance of the tunnel gap is reduced from 110 to 25 MΩ, the maximum amplitude at a fixed resistance decreases from 0.6 to 1.4 Å. At a constant resistance, however, it may vary by a factor of several units. Moreover, δz may change abruptly in the course of a given experiment (the average distance z remains essentially the same when this occurs). Near the top in Fig. 2a, we thus see no atomic structure at all. It disappeared in the transition from one scanning line to another. This result probably corresponds to a change in the configuration of the end of the tip upon the random capture or loss of individual atoms from the surface of the sample as these atoms diffuse over the tip.

In the case of lead, the corrugation amplitude on the STM images may thus exceed 1 Å. On the other hand, one might present an argument against the idea that the amplification results from a mechanical interaction. In the course of experiments we modulated the position of the sample along the z direction at a frequency ~ 2 kHz, exceeding the speed of the feedback, in order to monitor the purity of the surface. The modulation amplitude of the tunneling current became comparable to the current itself in this case, with a peak-to-peak value $z_v \approx 0.5$–1 Å. This value is close to that which would be expected on the basis of the known work functions of lead and tungsten (the tip material). If we assume, say, a van der Waals interaction, we can easily estimate that, if the mechanical stiffness of the system is low enough that a tenfold amplification of the observed atomic corrugation arises, then at a sample-tip distance on the order of an interatomic distance it would be necessary to raise z_v by the same order of magnitude (or more) in order to see the modulation of the tunneling current.

Ciraci *et al.*[10] have shown that an amplification may be caused by a restructuring of the electron wave functions in the gap due to an interaction of atoms of the tip with atoms of the sample surface. However, in contrast with the experiments of Refs. 3, 6, and 7, in which δz became greater than 0.3 Å at tunnel-gap resistances $R < 10$ MΩ, in our case this amplitude is realized at $R \approx 100$ MΩ. Since R characterizes the overlap of wave functions, it appears that we need to seek some mechanism for the phenomenon other than that proposed by Ciraci *et al.*[10]. In this connection, we would like to call attention to a calculation carried out by Chen *et al.*[11]. According to that calculation, the amplitude of the thermal vibrations of surface atoms becomes comparable to interatomic distances at a temperature as low as half the melting point. It must be kept in mind that, by analogy with the case of the tunneling of electrons from liquid helium into vacuum,[12] an exponentially decaying probability for finding the atom at a distance from the surface significantly greater than the average amplitude of the thermal vibrations is covered by an increasing probability for tunneling. Accordingly, atoms which have moved far away from their average position dominate the tunneling current. We might therefore expect that large values of δz in lead would be due to thermal motion.

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