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Atomic-scale connective neck formation and characterization

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A scanning tunneling microscope is used to form a connective neck of atomic size between a lead substrate and a lead tip. The elongation and contraction of the neck results in a regular and reproducible staircase structure in the tip-substrate conductance vs tip-displacement curve, giving physical insight on the plastic and elastic deformation mechanisms involved in atomic-scale structures.

Understanding the processes that occur when two materials are brought into contact in an atomic scale is of fundamental importance to problems such as adhesion, contact formation, surface deformations, plastic and elastic response of materials, materials hardness, friction and wear, and fracture.[1] Except in the case of atomically flat surfaces, contact is typically established at asperities or protrusions of very small size whose mechanical properties are known to be different to the corresponding bulk properties.[2] The scanning tunneling microscope (STM) and the atomic force microscope can be used not only to study contact formation on the atomic scale and to perform experiments with a single asperity or a contact of few atoms,[1,3,4] but to manipulate matter on the atomic scale.[5] On the other hand, large-scale molecular-dynamics simulations offer the possibility of studying the evolution of a system of interacting particles with high spatial and temporal resolution by direct integration of the equations of motion of the particles.[1,6] These studies simulate contact formation between a metal tip and a metal substrate. Changes in the area of the contact occur by sudden structural transformations, that cause abrupt changes in the force[1] and in the conductance.[6] As the tip is receded after indentation, a connective neck, which elongates in steps, by simultaneously changing its diameter and increasing the number of atomic planes in the neck, is formed.

In this paper we study the formation and characterization of the connective neck formed upon separation after the indentation of a metal substrate by a metal tip using STM. Both tip and sample are polycrystalline lead and the experiment was performed at 4.2 K; therefore lead is in the superconducting state. The low-temperature STM unit has been described elsewhere.[7]

Before indentation the substrate is scanned in order to locate an adequate clean area. The cleanliness of the surface can be assessed by measuring the apparent tunneling barrier.[3] Once on the selected spot, the tip is advanced towards the substrate while the current is monitored at fixed bias voltage. The point of first contact is easy to recognize because it is marked by the jump-to-contact phenomenon[1] which for a clean surface always takes place for a tip-to-substrate resistance of about 10 kΩ.[8] After contact is established the resistance depends on the area of the contact. For a circular contact of radius a, smaller than the mean free path l, the resistance is given by[9]

$$R = 4\rho l/3\pi a^2, \tag{1}$$

where ρ is the resistivity.

If we subject the substrate to a deep indentation and then recede the tip while moving it back and forth with a smaller amplitude, without breaking the contact, a reproducible and regular structure in the current vs tip-displacement curves develops. A typical example is shown in Fig. 1. In this case the tip was cyclically advanced and receded 47 Å starting from the right of the figure. Two complete cycles have been plotted to show the regularity and reproducibility of the staircase structure. These curves show a clear hysteresis: the curves corresponding to the advancing stage are always below those corresponding to the receding stage. The steps of the receding and advancing curves correspond to the same values of the current, but they occur for different tip displacements. The length of the steps is quite regular but different for both stages: 2.95 Å for the advancing stage and 2.65 Å for the receding stage. We have measured this step length for about 500 such curves obtained at

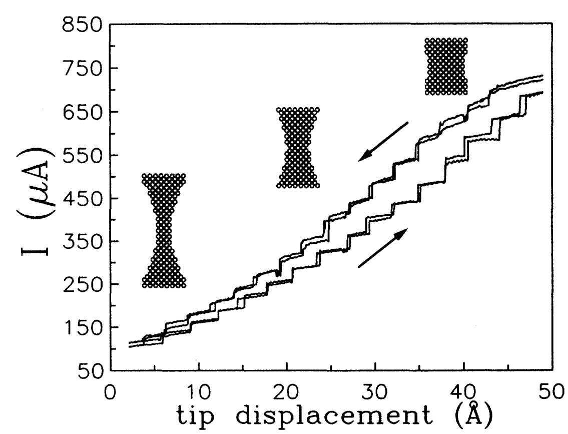

FIG. 1. Conductance of a neck obtained by repeated indentation of a lead substrate with a lead tip. Two curves for the approaching stage and two for the receding stage have been represented to show the degree of reproducibility. The bias voltage was 50 mV. The shape of the necks for the initial, final, and intermediate positions, computed as explained in the text, are also shown.

different spots. The average length of the steps is about 2.5 Å when the tip is receding and about 3 Å when it is advancing, as shown in the histogram of Fig. 2.

It is possible to obtain information about the shape of the connective neck formed between the tip and the substrate, from the variation of current with tip displacement, taking into account that the resistance of the contact depends on the narrowest section of the neck as given by Eq. (1). The experimental current vs tip displacement curves can be modeled assuming that only the material around the indentation takes part in the formation of the neck,[1] i.e., the volume of the neck is constant, and that the shape of the neck is parabolic. The shapes of the neck for maximum, intermediate, and minimum elongations are shown in Fig. 1. A disposition of atoms corresponding to a (001) layer (nearest-neighbor distance 3.5 Å) has been depicted to give an idea of the dimensions and number of atoms in the neck.

The molecular-dynamics simulations of Landman *et al.*[1] show that receding a nickel tip after indentation of a gold substrate results in the formation and elongation of a connective neck between tip and substrate due to the adhesive bonding between them resulting from intermetallic forces. The mechanism of elongation of this neck involves atomic structural transformations whereby in each elongation step atoms in adjacent layers in the neck disorder and then rearrange to form an added layer, that is, a more extended neck of a smaller cross-sectional area. These elongation steps consist of two distinct stages: an elastic stage, during which the force increases and the cross section of the neck is constant; and a yielding stage, in which the structural transformation takes place and, as a consequence, part of the force relaxes suddenly while the cross section of the neck decreases. These steps occur at rather regular tip-displacement intervals, whose average length is about 2 Å, which corresponds to the interlayer spacing between (001) layers of bulk gold. Throughout the process the neck maintains a layered crystalline structure except for the rather short structural transformation periods. On the other hand, the calculations of Todorov and Sutton[6] show that these structural transformations

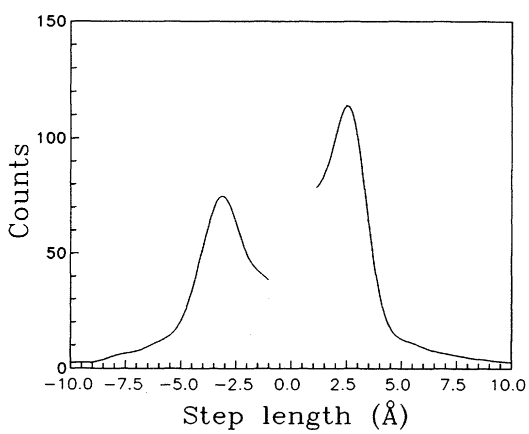

FIG. 2. Histogram of the step length, for about 500 different necks. Negative values are for the approaching stage, and positive values for the receding stage. Step length increments have been taken 0.125 Å wide.

cause abrupt changes in the conductance, and that the main factor controlling the conductance is the area of the contact while perturbations of the internal structure of the tip are of secondary importance.

The staircase structure in the experimental current vs tip displacement curves (Fig. 1), and the average step length, which is of the order of the interlayer spacing between (001) layers of bulk lead (2.5 Å), are consistent with the molecular-dynamics simulations.[1,6] Our results also show that the mechanism of contraction of this crystalline neck is the same as the mechanism of elongation described above, involving structural transformations that reduce the number of atomic layers in the neck while simultaneously increasing its cross section. The hysteresis and the difference in the step length between the advancing and receding stages (which is also observed in the calculations[6]), can be explained taking into account the macroscopic elastic deformation at the contact. According to Hertz theory for a contact between bodies of revolution the maximum macroscopic elastic deformation at a contact, before the onset of plastic deformation, is proportional to the radius of the contact.[10] During the advancing stage, when the neck is under compressive force, the macroscopic elastic deformation increases as the current increases. Thus, the macroscopic elastic deformation would be larger, the larger the current. The experimentally observed step length would be given by the tip displacement needed to contract the neck by one layer plus the increase in macroscopic elastic deformation due to the increase in contact radius caused by the structural transformation. During the receding stage, the neck is under tensile force and the macroscopic elastic deformation would be also larger, the larger the current, but in the *opposite direction* than for the advancing stage. In this case, the step length would be given by the tip displacement needed to elongate the neck by one layer minus the decrease in macroscopic elastic deformation due to the decrease in contact radius caused by the structural transformation. The regularity and reproducibility of the elongation and contraction processes clearly indicate the crystallinity of the neck.

Imaging the indented area after breaking the neck shows a protrusion whose size ranges from 80 to 300 Å, depending on the extent of the indentation. Typically, the height of the protrusion equals its diameter.

Many interesting physical phenomena originate in electronic transport through small-size constrictions joining two electronic reservoirs in the normal[11] as well as in the superconducting state. In the case of superconductors, these constrictions, known as point contact weak links have a number of desirable features from the point of view of the applications[12] but a very serious drawback is its lack of reproducibility and poorly defined geometry. The connective necks described in this paper clearly overcome these problems, making possible the study of superconducting structures down to atomic size. The study of conductance quantization[8] and the superconducting properties of variable size weak links is in progress in our laboratory.[13]

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