RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 47, NUMBER 18 1 MAY 1993-II

Conductance steps and quantization in atomic-size contacts

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(Received 18 February 1993)

The conductance of metallic contacts of atomic size has been studied using a scanning tunneling microscope at low temperature. As the contact area is changed by pressing the tip into the sample, a series of reproducible features and jumps in the conductance at integer multiples of $2e^2/h$ is observed. The jumps are interpreted as atomic rearrangements, while the underlying conductance structure strongly suggests quantum-size effects.

The capability of the scanning tunneling microscope (STM) to study the electrical conduction through very narrow constrictions was demonstrated by Gimzewzki and Möller.[1] These authors studied the tip to sample distance dependence of the electrical current in the transition from the tunneling regime to point contact. The contact between a tungsten tip and a silver sample was found to initiate with the intimate contact of only a few atoms. Dürig, Züger, and Pohl[2] investigated the interactions between an Ir tip and an Ir sample, measuring not only the resistance but also the interaction force between both electrodes and the onset of metallic adhesion. In these two experiments, an abrupt change in resistance was observed as the conduction regime changed from tunneling to point contact.

The possibility of observing quantization effects in the conductance[3] in STM point contacts as the tip is pressed against the sample has been discussed by several authors.[4,5] Quantum-size effects, due to the quantization of transverse momentum in the constriction, would be important for constriction diameters of the order of the Fermi wavelength. When the radius of an electrical contact or constriction between two metals is small compared to the mean free path of the electrons, the electrons are accelerated due to the electric field caused by the applied voltage, and are injected from one metal side to the other by passing through the contact. The transport of electrons is then said to be ballistic. Using a semiclassical treatment Sharvin[6] showed that the conductance of such a contact is independent of any material properties and is solely determined by the geometry of the contact and electron density, depending linearly on the contact area, $G_S = 3\pi a^2/4\rho l = (2e^2/h)k_F^2 a^2/4$, where a is the radius of the contact, l is the electron mean free path, and k_F is the Fermi wave vector.

A full quantum treatment[4,5] shows that the conductance is not linear in the area of the contact, but presents superimposed oscillations due to quantum interference effects even in the limit of a very short constriction. If the length of the constriction is of the order of the Fermi wavelength, λ_F, these quantum oscillations evolve into a steplike structure, with steps at integer multiples of $2e^2/h$. The effect of different confining potentials, scattering, and temperature has been the object of detailed study.[4,5]

Quantum-size effects have been observed in a two-dimensional electron gas. The conductance shows clear plateaus at integer multiples of $2e^2/h$ (Ref. 7) when the gate voltage controlling the width of the aperture is continuously varied.

Normal and superconducting small metallic constrictions have been studied recently by Muller, van Ruitenbeek, and de Jongh.[8] The observed irregular jumps in conductance were attributed to changes in the constriction involving a few atoms.

The ability of STM to vary the contact area in a controlled manner in atomic-size increments has been exploited in the study of several effects related to weak and nonequilibrium superconductivity.[9] We were able to obtain information about the different conduction regimes when the resistance of the junction formed by a superconductor and a normal metal changed from several megaohms down to a few ohms.

In this paper we present the experimental results obtained with small metallic point contacts of Au and Pb. In all reported measurements tip and sample were of the same material, and the temperature was 4.2 K. We used the same setup as in Ref. 9 with several minor modifications that improved the characteristics of our low-temperature STM. There was a stability of the order of 0.2 Å in the tunneling regime, without feedback for extended periods of time (several seconds). A triangular signal was applied to the z piezo, causing the tip to move perpendicular to the surface of the sample. The offset and amplitude of this signal were set in such a way that the tip moved from tunneling to contact beyond the point of contact formation while the current was recorded at fixed bias voltage. In both materials we formed many different point contacts on different spots of the sample taking advantage of the STM characteristics. Before touching the sample the contact area was scanned and the apparent barrier height (derivative of the logarithm of current with distance) was measured in order to ensure that the surface was clean.[1] Typical values for the probed spots were 4 eV for the Au sample and 3 eV for the Pb sample. The reported results are representative of the general behavior of the sample and not of a particular spot.

Figure 1 shows the conductance variations for Au tip and sample as a function of time. The amplitude of the

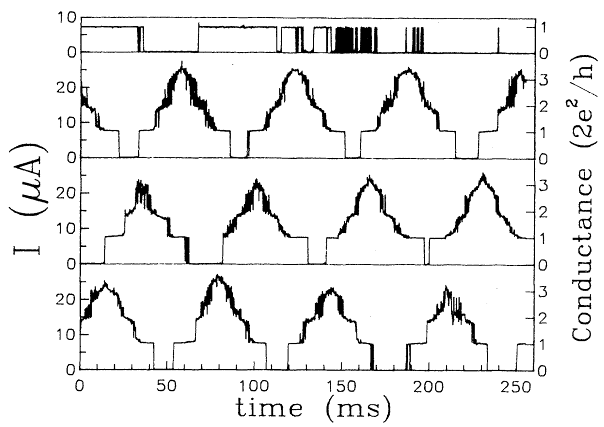

FIG. 1. Conductance variations for the Au point contact as the size of the constriction is varied. Bias voltage is fixed at 0.1 V. (a) Current (conductance) as a function of time. In the uppermost plot the z-piezo voltage is kept constant, note that the conductance oscillates by itself between two well-defined values, before the tip finally drifts away. In the other three plots the z-piezo voltage is scanned with a triangular signal of an amplitude of 1.5 V and a frequency of about 16 Hz (corresponding to a tip displacement of 14 Å). Note also that the conductance in the tunneling regime is negligible in the scale of the figure.

z-piezo movement is 14 Å. Before touching the surface of the sample the variation of the current is exponential but in the scale of the figure is negligible. As the tip approaches the substrate the current jumps by a factor of 10–20, and conductance attains a value of about $75 \pm 3 \times 10^{-6}\ \Omega^{-1}$ (the conductance quantum unit is $2e^2/h = 77.5 \times 10^{-6}\ \Omega^{-1}$). This jump in the conductance when the tip touches the sample is normally observed in STM experiments,[1,2] with a typical value of the resistance after the jump of about 10 kΩ. Molecular dynamics simulations of contact formation for Au-Ni and Au-Au systems[10] show that in response to the imbalance between the forces on atoms in each of the materials and those due to intermetallic interactions a jump-to-contact phenomenon occurs which involves the atoms in the interfacial region of the tip and substrate. This behavior depends on the mechanical properties of the material. For Au tips or substrate, displacements of about 2 Å are observed.

The fact that we *always* observe the same value of conductance, one quantum unit, after the jump-to-contact (see Fig. 1) seems to indicate that this process opens the first ballistic channel, and that the resulting contact is a one-atom contact. If one atom were not enough to open one ballistic channel, after the jump-to-contact the conductance would be due to tunneling and its value less than one quantum unit.[4] Furthermore, the displacement of the atoms after the jump-to-contact could result in a *longer* effective constriction, favoring a sharper quantization.[4,5]

As is shown in the top row of Fig. 1, it is possible to maintain the tip atoms oscillating between two positions in the vicinity of the jump-to-contact. The resulting conductance switches between two well-defined values, corresponding to different regimes: tunneling and ballistic. The high conductance state, with a conductance of one quantum unit, is very stable against tip displacements (3–5 Å) *beyond* the jump-to-contact (see the three lower rows in Fig. 1). The conductance of the low conductance state varies exponentially with distance, but attains a maximum value of only 0.06 quantum units right *before* the jump-to-contact. Consequently, it is very easy to select any of these two well-defined stable states by tip displacements of 3–5 Å. Positions closer to the jump-to-contact give rise to switching between these two states.

As the tip is further moved towards the sample, a somewhat regular structure is noticeable in the conductance both for advancing and receding motion of the tip. The theoretical works mentioned above[4,5] indicate that the conductance vs area variations for our experimental geometry (short constriction and finite temperature) would be in the form of a smooth staircase, with steps for integer multiples of the quantum conductance unit, that smears out as the conductance increases. The length of the steps and of the transition region between the steps would depend strongly on the exact shape of the potential at the constriction.[4] In order to understand this structure in the conductance, it is necessary to consider how the changes in the tip position affect the geometry of the contact. Area variations are caused by rearrangements of the few atoms involved in the contact; any sudden variation would cause a jump in the conductance, of the order of one quantum unit (since one atom is enough to open a ballistic channel). Obviously, any structure of the conductance curves would be distorted by such sudden area variation. Distortions of the conductance curves may also result from elastic deformations of the tip or substrate that would show as sample plateaus. This effect can be clearly observed in the first plateau (from 3 to 5 Å long, and conductance of one quantum unit) corresponding to the elastic recovery of the tensile deformation produced by the jump to contact.

If distortions, both in conductance and in displacement, due to sudden atomic rearrangements (jump-to-contact, elasticity) are taken into account, we recognize in these curves the smooth staircase structure due to quantization effects (with steps for 1, 2, and 3 quantum units signaling the opening of new ballistic channels) predicted by the theory.[4,5] For larger z-piezo movement amplitudes, it is difficult to discern further steps due to the smearing of the staircase structure as the number of channels increases.

Figure 2 shows the results for lead point contacts. Sharp jumps corresponding to atomic rearrangements (one of them shows hysteresis) superposed to a smoother structure are evident in the conductance. As explained above, such a smooth structure with slight inflections for integer values (for example, at 1,3,5 quantum units) of the conductance would result from quantum-size effects. The differences in behavior between gold and lead could be due to the difference in the mechanical properties of both materials[11] and in the geometry of the tip, which seems to be blunter in the case of Pb (worse resolution when scanning).

The fact that lead is a superconductor offers the possi-

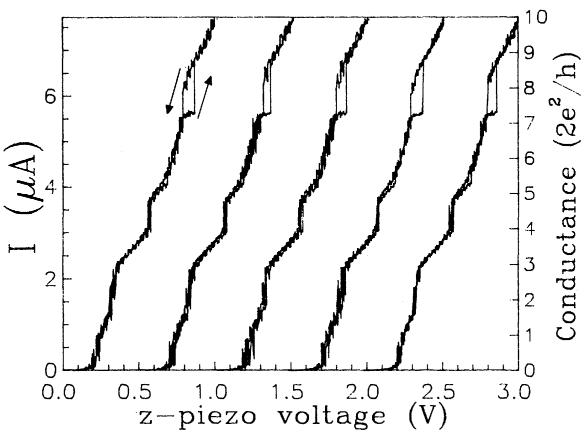

FIG. 2. Conductance variations for the Pb point contact as the size of the constriction is varied. The z-piezo voltage was scanned as explained for Fig. 1, the amplitude was about 1 V (corresponding to 9.3 Å), and the bias voltage was fixed at 10 mV. The arrows indicate the scan direction. Each pair is displaced in horizontal axis, for clarity.

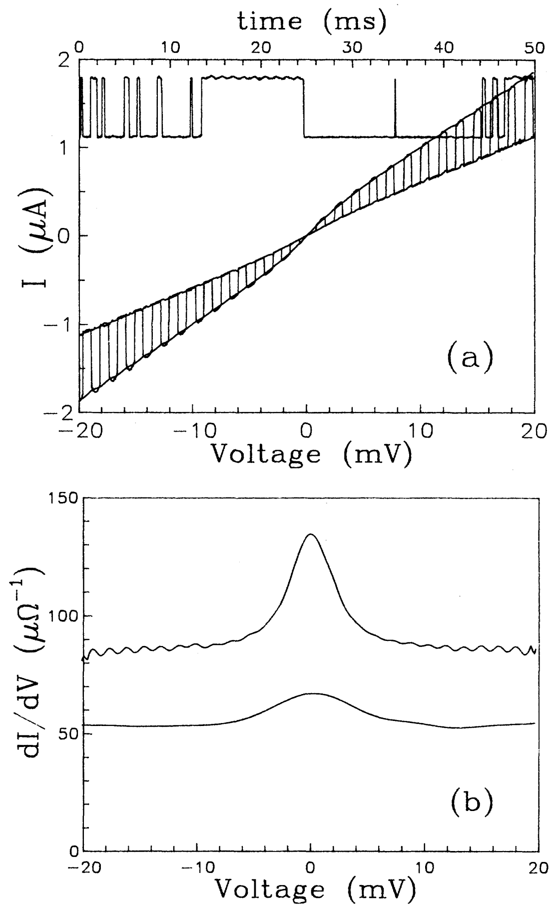

FIG. 3. Pb point contact. (a) The upper plot shows the current as a function of time when the z-piezo voltage is kept constant. Bias voltage is fixed at 20 mV. The tip jumps to contact but from a shorter distance than in the case of Au. The lower plot shows the I-V characteristic curve before and after the jump; bias voltage is ramped in about 30 ms (z-piezo voltage kept constant). (b) Differential conductance curves corresponding to the two I-V curves in (a).

bility of obtaining additional information about the evolution of the Pb point contacts.[9] The I-V characteristic curves and differential conductance curves in Figs. 3(a) and 3(b) show the conductance before and after the jump to contact. In Fig. 3(a), the jump is from $54 \times 10^{-6}\ \Omega^{-1}$ to $84 \times 10^{-6}\ \Omega^{-1}$. The shape of the curves indicates that the barrier was almost totally collapsed before the jump indicating very close proximity.[12] The jump to contact in the gold point contact was always from the tunneling regime. Acting on the z-piezo voltage it was possible to select one of these states. The normal conductance of the superconductor attains the value corresponding to one unit, but the current is larger due to the excess current caused by the Andreev reflection.[12]

In summary, we have studied the possibility of observing conductance quantization effects using a STM. Our results show that in spite of the fact that the contact area varies in atomic increments, which causes jumps in conductance of the order of $2e^2/h$, the smoother underlying structure at integer multiples of $2e^2/h$ in the conductance suggests quantum-size effects in the narrow constriction formed between the tip and the sample. Noteworthy is the possibility to control the switching between the tunneling and the ballistic conductance regimes, with conductances that differ in a factor of about 15 (in the case of Au), by slightly moving the tip.

We would like to thank C. Sirvent for his assistance in the improvement of our experimental setup. Discussions with J. J. Saénz, and N. García are gratefully acknowledged. This work has been supported by the Comunidad de Madrid under Contract No. C031/90, and by the CICYT under Contract No. MAT92.

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[11]The elastic modulus is 78 GPa for Au, and 16 GPa for Pb; the yield strength for Au is 200 MPa and for Pb is 5.5 MPa.

[12]The transition from the tunneling regime to point contact in a superconducting junction is marked by an increase in the conductivity for small biases due to Andreev reflection [see M. Octavio, M. Tinkham, G.E. Blonder, and T.M. Klapwijk, Phys. Rev. B **27**, 6739 (1983)]. A detailed study of this process using STM is made in Ref. 9. It must be remarked that in spite of the fact that we have a contact between two superconducting electrodes the observation of a supercurrent is not to be expected in Fig. 3(b), because the Josephson coupling energy for such a high resistance weak link is too small compared to thermal fluctuations. The conductance of the contact should be about ten times larger in order to observe a supercurrent, see for example, C.M. Falco, W.H. Parker, S.E. Trullinger, and P.K. Hansma, Phys. Rev. B **10**, 1865 (1974).