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Single-channel transmission in gold one-atom contacts and chains

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We induce superconductivity by proximity effect in thin layers of gold and study the number of conduction channels which contribute to the current in one-atom contacts and atomic wires. The atomic contacts and wires are fabricated with a scanning tunneling microscope. The set of transmission probabilities of the conduction channels is obtained from the analysis of the $I(V)$ characteristic curve which is highly nonlinear due to multiple Andreev reflections. In agreement with theoretical calculations, we find that there is only one channel that is almost completely open.

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Much effort has been devoted in the last decade to the understanding of electron transport processes and mechanical properties of atomic-sized point contacts and chains between metallic electrodes.[1] Coherent electron transport in these nanostructures can be understood in the frame of the scattering formalism. The conductance G of these nanocontacts is given by the Landauer formula $G=G_0\Sigma_{i=1}^{N}\tau_i$, where τ_i are the transmission probabilities for each of N conductance channels and $G_0=2e^2/h$ is the conductance quantum. For a given contact realization, the conductance channels are in general neither completely open nor completely closed and the transparency τ_i of each channel depends on the material forming the contact,[2,3] detailed atomic arrangement, and applied stress.[4] In this report we study the channel transparency set $\{\tau_i\}$ both in gold one-atom contacts and chains of single gold atoms,[5] for which theoretical models[4,6–9] predict an almost completely open single channel, and therefore a conductance close to G_0.

It is well established that conductance histograms (CH) show that the conductance of one-atom contacts of gold is close to G_0[1] but the values of τ_i cannot be obtained only from the measurement of the total conductance. However, the marked nonlinearity of the current-voltage characteristic (*IV*) of superconducting contacts has been exploited to obtain the set of transmission coefficients $\{\tau_i\}$ of atomic-sized aluminum contacts.[10] The channel transmission probabilities are extracted by fitting the measured *IV* curve to a sum of N independent *IV*'s calculated for individual channels with a given transmission probability.[11,12] This method was afterwards extended to other superconducting materials, showing that the number of conducting channels contributing to the current in one-atom contacts is limited by the valency of the atom at the contact.[2]

Gold is not superconducting. However, we take advantage of the superconducting correlations induced in a thin layer of normal metal in contact with a superconductor. The energy spectrum is modified and a gap is opened at the Fermi energy. At low voltages, transport is dominated by Andreev reflection processes which results in nonlinear *IV* curves. Here, we use the aforementioned method[2,10] to analyze the transmission coefficients of proximity induced superconducting one-atom contacts and atomic chains of gold.

The proximity effect has been previously exploited,[2,13] to get information of the $\{\tau_i\}$ in gold atomic contacts. In the first experiment[2] the *IV* curves were fitted to a sum of theoretical *IV*'s corresponding to BCS superconductors, and the contribution of a single channel in one-atom contacts is reported. However, the energy dependence of the density of states and the probability of Andreev reflection at a proximity-induced superconducting contact are blurred with respect to the BCS model.[14] The modifications due to the proximity character of the superconducting correlations were taken into account in the later experiment.[13] Most of the experimental *IV*'s recorded at the last conductance plateau before contact breaking could be fitted with a single channel. Several channels were necessary to fit the *IV* curves of some contacts with conductance smaller than G_0. However, in these experiments the conductance of the smallest contacts is usually much smaller than G_0, being the first peak of the histogram placed at $0.6G_0$ and plateaux not nearly flat. These results are not consistent with what has been usually reported in gold atomic contacts in the normal state.[1] Here we report experiments in which the conductance histograms for proximity superconducting gold and normal gold are in remarkable agreement (Fig. 1). We also study the channel content of chains of gold atoms.

Nanocontacts are produced by pressing two wires crosswise against each other. The wires are used as electrodes in place of a tip and sample of a scanning tunneling microscope. The separation and contact size between the wires can be controlled with the piezoelectric positioning system the microscope. The advantage of using two crossed wires is the possibility of selecting the position of the point contact along both wires using the coarse lateral displacement capability of the microscope, allowing for the exploration of point contacts at different spots along the wires. The wires (0.25 mm diameter) are made of bulk lead and are in the first preparation step covered by thermal evaporation with a thick layer of lead (900 nm at a rate of 0.8 nm/s). This thick layer of lead provides a clean surface. A thin layer of gold (28 nm, rate of 0.1 nm/s) is then evaporated on top of the Pb layer. The lead and gold deposition sequence is performed without breaking the vacuum in the chamber ($<10^{-6}$ mbar), thus preventing the presence of oxide at the Pb-Au interface and

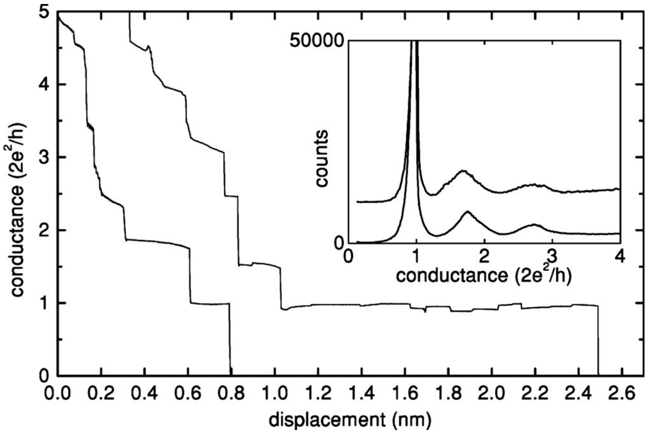

FIG. 1. Differential conductance at a bias voltage of 10 mV of proximity-induced superconducting gold contact during pull-off. One-atom contact formation (left) and atomic chain (right). The length of the conductance plateau indicates that a chain longer than five atoms is formed. Inset: conductance histograms of gold in the normal state (bottom) and proximity superconducting (shifted upwards 10 000 counts).

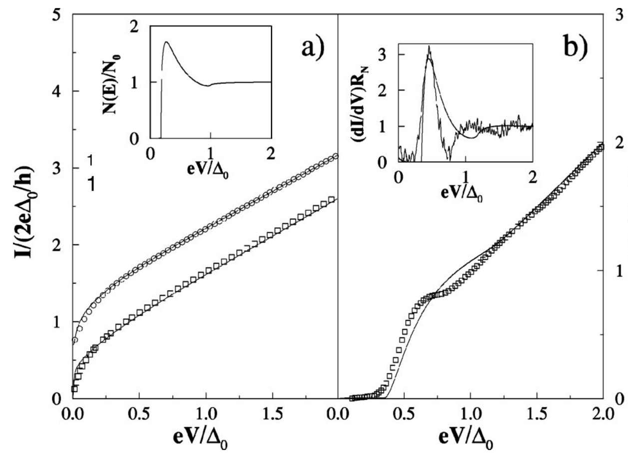

FIG. 2. Main figures show the *IV* curves corresponding to the tunneling regime (b), a single-atom contact [bottom curve in (a)] and an atomic chain [top curve in (b)]. The curve corresponding to the atomic chain has been displaced for clarity. Experimental results are shown by symbols and theoretical fittings by solid lines. The transmissions obtained in the contact regime are $T_1 = 0.995$ (single atom) and $T = 0.96$ (chain). Inset in (a) shows the density of states used to calculate the theoretical curves—see text. Inset in (b) shows the derivative of the experimental (the one with noise) and calculated tunneling curves.

ensuring good electrical contact between both layers. The substrate is at a temperature of 80 K during film deposition. One-atom contacts are fabricated by slight indentation (<3 nm) and subsequent retraction of the electrodes. Further retraction results in contact breaking and a jump to the tunneling regime. Experiments are done at 1.8 K. During nanocontact pull-off, the conductance trace is steplike (see Fig. 1). This characteristic behavior has been shown to be due to the mechanical processes that take place during contact breaking;[15] conductance plateaus corresponding to elastic deformation stages and sharp conductance changes related to sudden rearrangements of the atoms in the narrowest part of the nanocontact.

For gold nanocontacts in the normal state, the last conductance plateau before contact breaking is close to G_0 and corresponds to the smallest possible contact: a one-atom contact. Despite the inherent variability of the exact conductance trace during contact pull-off, it has been shown in several experiments that the CH over a large number of contact breaking realizations displays peaks at conductance values that are characteristic of the chemical nature of electrodes.[1] CH in gold nanocontacts have a characteristic first peak at a conductance close to G_0. We show in the inset of Fig. 1 a comparison between CH obtained for bulk gold tips in the normal state and in proximity induced superconducting gold nanocontacts. Due to the presence of excess current in the *IV*'s of superconducting nanocontacts, it is necessary to measure the differential conductance at a fixed bias voltage well above Δ/e, where Δ is the energy of the superconducting gap. The remarkable agreement between both CH's supports the validity of our analysis also for atomic-sized contacts of gold in the normal state. The low value of the conductance of the first peak in the conductance histogram in Ref. 13 was probably due to enhanced elastic scattering related to a sample preparation method.

We show in Fig. 2 representative *IV* curves recorded at a one-atom contact, in an atomic chain and in the tunneling regime, up to a voltage $2\Delta_0/e$, where $\Delta_0 = 1.40$ meV is the bulk superconducting gap for lead. We show both the measured *I-V* curves (symbols) and theoretical fitting (lines). The theoretical *IV*'s in the contact regime are calculated by solving the time-dependent Bogoliubov de Gennes equations within the scattering formalism.[11,16] This method requires the knowledge of the Andreev reflection amplitude of probability $[a(E)]$ at the contact, where the voltage drops. $a(E)$ can be computed if the normal and anomalous Green functions are known.[16] In the tunneling regime, the *IV*'s are calculated by the usual convolution of the densities of states at both sides of the barrier.[17]

As both Au-Pb electrodes are only very weakly coupled at the weak link, to calculate the density of states and the Andreev reflection amplitude of probability, we model our system as two independent normal-superconducting (NS) structures and solve self-consistently the Usadel equations.[14,18] Usadel equations provide a quasiclassical description of the Green functions of a superconductor in the dirty limit, in which electronic transport is diffussive. Elastic impurity scattering is included in the Born approximation and is characterized by a mean free path l (or a diffusion coefficient $D = v_F l/3$). A description based on Usadel equations was recently used to explain the *IV* curves of lead nanostructures under the influence of a magnetic field and proximity effect, providing excellent quantitative agreement with experiment both in the contact and tunneling regimes.[19,20]

The two NS are assumed to be equal and consist of a dirty normal layer with thickness d_N which is bounded at one end by vacuum and joined to a dirty semi-infinite superconductor at the other. Note that the diffussive description is expected to be valid in the case $d_N \ll l$. The Green functions that are relevant to calculate the IV curves are the ones at the vacuum-bounded edge of the normal layer. The proximity effect is also affected by the existence of a barrier at the interface as quasiparticles normally reflected do not contribute to it. In a diffusive system, the mismatch between the characteristic parameters (conductivity and diffusion coefficients) of the normal and superconducting metals leads to an effective barrier for the quasiparticles. It can be described through the parameter $\Gamma=(D_S/D_N)^{1/2}\sigma_N/\sigma_S$. In our model we assume $\Gamma=1$ and a vanishing resistance of the interface.[21] With these assumptions, the superconducting correlations in the normal metal are described by Δ_0 and the value of d_N/ξ_S, where ξ_S is the coherence length of the superconductor. In the atomic chain and one-atom contact, the transmission channels set enters also as fitting parameters. A similar model was used by Scheer *et al.*[13] in the description of Au contacts with superconductiviy induced by proximity effect. In their case, however, the mismatch parameter Γ was also used as a fitting parameter.

Solid lines in Fig. 2 show the calculated *IV* which for the same sample fitting parameter, $d_N/\xi_S=0.81$, best fit both the curves in the tunneling and the contact regime. Assuming the nominal thickness $d_N=28$ nm it corresponds to a superconducting coherence length $\xi_S=34$ nm, in good agreement with the values obtained in Refs. 19 and 20.

The tunneling regime *IV* curve, plotted in Fig. 2(b), shows a gap smaller than Δ_0 and a bump characteristic of NS structures.[22] It is however poorly fitted,[23] which means that the density of states used, shown in the inset of Fig. 2(a), does not agree completely with the experimental one. The source of disagreement in the fitting can be better understood by looking at the derivative of the experimental and theoretical tunnel *IV* curves, shown in inset in Fig. 2(b). The theoretical curve shows an asymmetric peak at the gap which decays slowly as the energy increases and results from the one in the density of states. This asymmetric peak structure is characteristic of the diffusive regime for parameters that give gaps in the normal metal much smaller than Δ_0. The peak in the experimental curve is more symmetric. More rounded peaks (and tunneling curves with a bump more similar to the one obtained experimentally) can be obtained for much smaller values of d_N/ξ_S. In the diffusive regime, the gap induced in the spectrum of the normal metal decreases with d_N/ξ_S. Lower values of the fitting parameter induce gaps with values much closer to Δ_0 and could not explain the strong reduction of the gap found experimentally and would give worse fits.

Scheer *et al.*[13] also found disagreement in the fit of the tunneling conductance and related it to the nondiffusive character of the samples, being the condition $d_N \ll l$ not fulfilled. The proximity effect is a consequence of the coherent superposition of Andreev reflection and is strongly influenced by the length of the path that the electron travels between Andreev reflection processes. Thus, the energy dependence of the induced pair correlations is very sensitive to the degree of disorder in the normal metal and the shape of the spectrum differs considerably in the clean and dirty limits.[14,22,24] We have also tried, without success, to fit the experimental curves assuming that there is no disorder, the transport in the electrodes being ballistic, instead of diffusive.[22,24–26] As concluded by Scheer *et al.*,[13] we think that the lack of good fittings in the tunneling regime is due to transport in the gold layer being in the weakly disordered regime, instead of in the diffusive or clean limits.

Given the uncertainty in the density of states, the accuracy with which the channel transmission set is obtained in the contact regime is slightly reduced, compared to the ones done in BCS superconductors. The single-atom curve can be reasonably well fitted with a very open channel with transmission $T_1=0.995$. The chain is reasonably well fitted by a single channel with transmission $T=0.96$. This result is representative of the general behavior that we observe thus confirming that one widely open channel is responsible for the conduction in single-atom gold contacts, in agreement with theoretical predictions.[6–9]

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[1] N. Agraït, A. Levy-Yeyati, and J.M. van Ruitenbeek, Phys. Rep. (to be published).

[2] E. Scheer, N. Agraït, J.C. Cuevas, A. Levy Yeyati, B. Ludoph, A. Martín-Rodero, G. Rubio-Bollinger, J.M. van Ruitenbeek, and C. Urbina, Nature (London) **394**, 154 (1998).

[3] C. Sirvent, J.G. Rodrigo, S. Vieira, L. Jurczyszyn, N. Mingo, and F. Flores, Phys. Rev. B **53**, 16 086 (1996).

[4] J.C. Cuevas, A. Levy-Yeyati, A. Martín-Rodero, G. Rubio-Bollinger, C. Untiedt, and N. Agraït, Phys. Rev. Lett. **81**, 2990 (1998).

[5] A.I. Yanson, G. Rubio-Boliinger, H.E. van den Brom, N. Agraït, and J.M. van Ruitenbeek, Nature (London) **395**, 780 (1998); H. Ohnishi, Y. Kondo and K. Takayanagi, *ibid.* **395**, 783 (1998).

[6] J.C. Cuevas, A. Levy-Yeyati, and A. Martín-Rodero, Phys. Rev. Lett. **80**, 1066 (1998)

[7] T. López-Ciudad, A. García-Martín, A.J. Caamaño, and J.J. Sãenz, Surf. Sci. Lett. **440**, L887 (1999).

[8] M. Brandbyge, J.L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro, Phys. Rev. B **65**, 165401 (2002); S.K. Nielsen, M. Brandbyge, K. Hansen, K. Stokbro, J.M. van Ruitenbeek, and F. Besenbacher, Phys. Rev. Lett. **89**, 066804 (2002).

[9] J.J. Palacios, A.J. Pérez-Jiménez, E. Louis, E. SanFabian, and J.A. Vergés, Phys. Rev. B **66**, 035322 (2002); Note that while in this work a conductance larger than one quantum and the contribution of three channels is predicted, one of these channels is almost completely transmitting. The single-channel conductance is recovered for atomic chains.

[10] E. Scheer, P. Joyez, D. Esteve, C. Urbina, and M.H. Devoret, Phys. Rev. Lett. **78**, 3535 (1997)

[11] D. Averin and A. Bardas, Phys. Rev. Lett. **75**, 1831 (1995).

[12] J.C. Cuevas, A. Martin-Rodero, and A. Levy-Yeyati, Phys. Rev. B **54**, 7366 (1996).

[13] E. Scheer *et al.*, Phys. Rev. Lett. **86**, 284 (2001).

[14] W. Belzig, C. Bruder, and G. Schön, Phys. Rev. B **54**, 9443 (1996).

[15] G. Rubio, N. Agraït, and S. Vieira, Phys. Rev. Lett. **76**, 2302 (1996).

[16] A.V. Zaitsev and D.V. Averin, Phys. Rev. Lett. **80**, 3602 (1998).

[17] *Introduction to Superconductivity*, edited by M. Tinkham (McGraw-Hill, New York, 1996).

[18] K.D. Usadel, Phys. Rev. Lett. **25**, 507 (1970).

[19] H. Suderow, E. Bascones, W. Belzig, F. Guinea, and S. Vieira, Europhys. Lett. **50**, 740 (2000).

[20] H. Suderow, E. Bascones, A. Izquierdo, F. Guinea, and S. Vieira, Phys. Rev. B **65**, 100519 (2002).

[21] We have found that to introduce the influence of the mismatch of the Fermi velocities and mean free path in gold and lead or of an interface resistance does not improve significantly the quality of the fittings and would introduce more fitting parameters.

[22] G.B. Arnold and E.L. Wolf, Phys. Rev. B **25**, 1541 (1982).

[23] A slightly better agreement can be obtained with a larger d_N/ξ. Larger values of d_N/ξ do not fit properly the *IV* curve in the contact regime for any value of the channels transmission.

[24] G.B. Arnold, Phys. Rev. B **18**, 1076 (1978)

[25] E. Vecino, A. Martin-Rodero, and A. LevyYeyati, Phys. Rev. B **64**, 184502 (2001)

[26] G. Kieselmann, Phys. Rev. B **35**, 6762 (1987)