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 non-linear due to multiple Andreev reflections. In agreement with theoretical calculations we find that there is only one channel which 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. 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 $G = G_0 \sum_{i=1}^{N} \tau_i$, where $\tau_i$ are the transmission coefficients for each of $N$ conduction 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 $\tau_i$ of each channel depends on the material forming the contact, detailed atomic arrangement and applied stress. In this report we study the channel transparency set $\{\tau_i\}$ both in gold one-atom contacts and chains of single gold atoms, for which theoretical models 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 $G_0$ but the values of $\tau_i$ cannot be obtained from the only measurement of the total conductance. However, the marked non-linearity of the current-voltage characteristic ($I(V)$) of superconducting contacts has been exploited to obtain the set of transmission coefficients $\{\tau_i\}$ of atomic-sized aluminum contacts. The channel transmission probabilities are extracted by fitting the measured $I(V)$ curve to a sum of $N$ independent $I(V)$s calculated for individual channels with a given transmission probability. 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 valence of the atom at the contacts.

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 non-linear $I(V)$ curves. Here we use the aforementioned method to analyze the transmission coefficients of proximity induced superconducting one-atom contacts and atomic chains of gold.

The proximity effect has been previously exploited to get information of the $\{\tau_i\}$ in gold atomic contacts. In the first experiments the $I(V)$ curves were fitted to a sum of theoretical $I(V)$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 smeared with respect to the BCS model. The modifications due to the proximity character of the superconducting correlations were taken into account in the later experiments. Most of the experimental $I(V)$s recorded at the last conductance plateau before contact breaking could be fitted with a single channel. Several channels were necessary to fit the $I(V)$ 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 0.6 $G_0$ and plateaux not nearly flat. These results are not consistent with what has been usually reported in gold atomic contacts in the normal state. 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 tip and sample of an STM. The separa-
tion 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 a 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 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 step-like (see Fig. 1). This characteristic behavior has been shown to be due to the mechanical processes that take place during contact breaking; 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 conductance histogram (CH) over a large number of contact breaking realizations displays peaks at conductance values that are characteristic of the chemical nature of electrodes. 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 IVs of superconducting nanocontacts it is necessary to measure the differential conductance at a fixed bias voltage well above \( \Delta/e \), where \( \Delta \) is the energy of the superconducting gap. The remarkable agreement between both CH 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 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 IV curves (symbols) and theoretical fitting (lines). The theoretical IVs in the contact regime are calculated by solving the time-dependent Bogoliubov de Gennes equations within the scattering formalism. 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. In the tunneling regime the IVs are calculated by the usual convolution of the densities of states at both sides of the barrier.

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. Usadel equations provide a quasiclassical description of the Green functions of a superconductor in the dirty limit, in which electronic transport is diffusive. 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 regime.

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 diffusive description is expected to be valid in the case \( d_N \ll l \). The Green functions which are relevant to calculate the IV curves are the ones at the vacuum-bounded edge of
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) show the derivative of the experimental (the one with noise) and calculated tunneling curves.

the normal layer. The proximity effect is also, affected by the existence of a barrier at the interface, as quasi-particles 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. With these assumptions the superconducting correlations in the normal metal are described by $\Delta_0$ and the value of $d_N/\xi_S$, where $\xi_S$ 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.\textsuperscript{13} in the description of Au contacts with superconductivity induced by proximity effect. In their case, however, the mismatch parameter $\Gamma$ 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 Ref.\textsuperscript{13} and\textsuperscript{20}.

The tunneling regime $IV$ curve, plotted in Fig. 2b, shows a gap smaller than $\Delta_0$ and a bump characteristic of NS structures\textsuperscript{23}. It is however poorly fitted\textsuperscript{26}, 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 which give gaps in the normal metal much smaller than $\Delta_0$. 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 $d_N/\xi_S$. In the diffusive regime the gap induced in the spectrum of the normal metal decreases with $d_N/\xi_S$. Lower values of the fitting parameter induce gaps with values much closer to $\Delta_0$ and could not explain the strong reduction of the gap found experimentally and would give worse fits.

Scheer et al.\textsuperscript{13} also found disagreement in the fit of the tunneling conductance and related it to the non-diffusive 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 which 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 shape of the spectrum differs considerably in the clean and dirty limits\textsuperscript{15,22,23}. We have also tried, without success, to fit the experimental curves assuming that there is no disorder being the transport in the electrodes ballistic, instead of diffusive\textsuperscript{22,23,24,25}. As concluded by Scheer et al.\textsuperscript{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\textsuperscript{6,7,8,9}.

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