Atomic-Sized Metallic Contacts: Mechanical Properties and Electronic Transport

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Measuring simultaneously the force and the conductance during the formation and rupture of an atomic-sized gold contact at room temperature, we observe that deformation occurs as a sequence of structural transformations involving elastic and yielding stages and that force and conductance before rupture have definite values which are likely to correspond to a single atom contact. We measure the mechanical properties of contacts consisting of only a few atoms and show that the stepwise variation of the conductance is always due to the atomic rearrangements in the contact.

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The mechanical and electrical behavior of small contacts between metallic bodies is at present a subject of intensive research [1–6]. It is accepted today that many macroscopic phenomena of crucial technological importance, such as adhesion, friction, wear, and fracture, have their origin in the combined action of many of these microscopic- and nanoscopic-sized contacts. Recently, it has been emphasized by Smith [7] the possible practical importance of the smallest of these structures as atomic-sized switches, which use as working principle the observed electrical conductance jumps in an atomic-sized contact.

In a previous work we characterized at liquid helium temperature nanometer-sized metallic contacts down to about 100 atoms [1]. The characterization included an experimental study of their mechanical behavior when submitted to compressive and tensile forces, in addition to a simultaneous study of the electronic transport. In this Letter, we present results on the mechanical and electrical properties of atomic-sized contacts at room temperature and ambient conditions using a modified setup.

The inset in Fig. 1(a) gives a schematic idea of the setup that is similar to the one used in Ref. [1]. A clean gold sample [8] is mounted at the free end of a cantilever beam. A piezoelectric transducer is used to control the distance between the gold tip and sample. The gold used is polycrystalline of 99.99% purity. A metallic atomic-sized contact is formed by touching the substrate with the tip. After this indentation the tip is retracted and a connective neck is formed, whose geometry changes as it is elongated and contracted [9]. The conductance is obtained measuring the current between the tip and the sample with an applied bias voltage (10 mV). The force is obtained measuring the deflection of the cantilever beam with an atomic force microscope (AFM) setup working in the contact mode. We use a home-built laser beam deflection detection AFM. The spring constant of the cantilever (5 mm × 2 mm) on which the gold sample is mounted is calibrated using weights and its resonant frequency is measured. When the AFM cantilever (100 μm long) is put into contact the new effective spring constant of the

combined system is obtained measuring the shift of the resonant frequency.
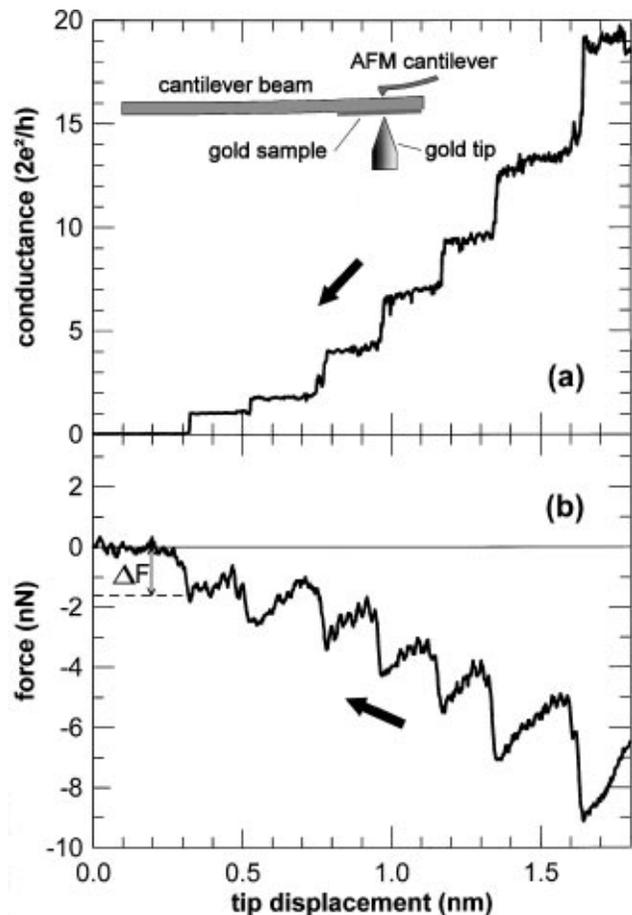
FIG. 1. Representative simultaneous recording of the measured conductance and force during the elongation of an atomic-sized constriction at 300 K. This constriction is elongated until rupture retracting the tip 1.8 nm (x axis). (a) The conductance during the deformation of the constriction is plotted in units of the conductance quantum ($2e^2/h$). (b) The simultaneous force sequence measured with a cantilever beam of effective spring constant 25 N/m. Inset: Experimental setup.

We show in Fig. 1 a simultaneous measurement of the electrical conductance and the force during the elongation of an atomic-sized neck that finally breaks. During the stretching of the neck the force follows a sequence of constant slope elastic stages and force relaxations due to atomic rearrangements [10,11]. The simultaneously measured conductance remains almost constant in the elastic stages, and there is an abrupt conductance change when the force relaxes. This behavior of the conductance has been predicted by molecular dynamics simulations [12]. From an analysis of ten curves showing a similar behavior to the curve in Fig. 1 we have found a value of the last conductance step of $G = 0.98G_0 \pm 0.07$ where $G_0 = 2e^2/h$ is the conductance quantum [13]. For gold this is the typical value for the last step of conductance [4,7,14]. This contact possibly consists of just one atom [4]. This idea is supported by the molecular dynamics simulations of Todorov and Sutton [12] that show that there is a one atom contact just before pulloff, and its electrical conductance is very near to the conductance quantum G_0. The force needed to break this last contact is obtained from the simultaneously measured force curves, and is also quite well defined $\Delta F = 1.5 \pm 0.2$ nN. This is the last force relaxation observed. The order of magnitude of this force is consistent with a rough estimate of the force necessary to pull an atom off a surface, obtained from a simple reasoning using the cohesive energy. For gold, the cohesive energy is 3.81 eV per atom, and assuming that on the surface an atom has three bonds instead of the twelve it has in the bulk, and that the range of the force is of the order of 0.1 nm, the force would be 1.6 nN.

A qualitatively different behavior of the conductance and force is observed in spots where the presence of contamination, as attested in both the approach and retraction force curves, is important. In these mechanical contacts conductance values much smaller than G_0 are normally observed. Recently it has been suggested that a similar conductance behavior observed during retraction in scanning tunneling microscopy (STM) experiments in ambient conditions [6] is due to electronic localization in an increasingly thinner metal wire. Our combined force and conductance measurements show that a more plausible interpretation of these results is in terms of conduction through the contamination layer.

In the experiment we perform repeated load cycles of contraction and subsequent elongation of the neck without breaking the contact. One of these cycles is shown in Fig. 2. For this kind of structure we can make an estimate of some mechanical parameters involved in the deformation. The maximum pressure that the neck can sustain before relaxation can be computed from the measured force and the contact area. This area is obtained from the measured conductance using a modified Sharvin equation [15]. This apparent pressure ranges from 3 to 6 GPa for both the compressive and tensile branches of the cycle, down to contact areas of 1.2 nm^2 characterized by a conductance of
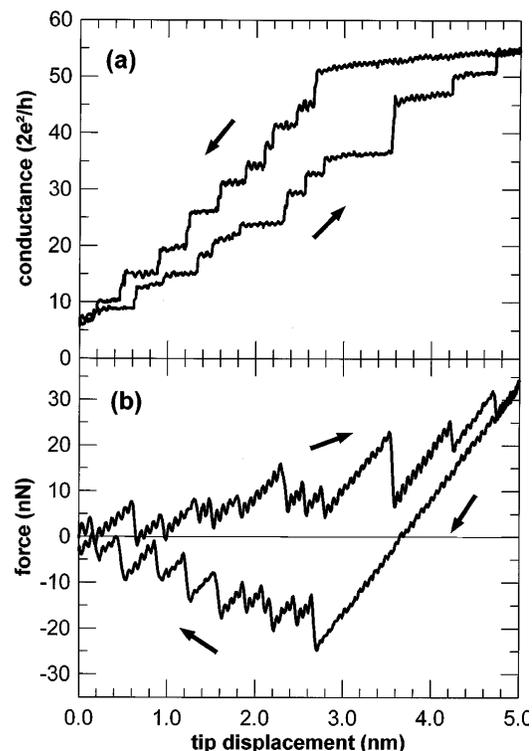
FIG. 2. Simultaneous recording of the conductance (a) and force (b) during a cycle of contraction and elongation of a constriction without breaking the contact. The effective spring constant of the cantilever beam used here is 35 N/m. The arrows indicate the direction of the tip displacement. The area of the contact given by the modified Sharvin equation goes from 0.9 to 6.9 nm^2.

10 quantum units [Fig. 3(a)]. Similar behavior has been observed in nanometer-scale contacts [1]. This apparent pressure is more than 20 times larger than the maximum pressure that a macroscopic contact can sustain [16], and is of the same order of magnitude as the theoretical value in the absence of dislocations [17]. The particular geometry of the constriction at the different stages during the deformation can explain the different values of the pressure from one point to another. Only for smaller contact areas this pressure increases up to 13 GPa for the smallest contact of one conductance quantum unit [Fig. 3(b)]. The deviation of the maximum apparent pressure before atomic rearrangements for the smaller contacts is to be expected since most of the constituent atoms are at surface positions, and surface energy effects become important.

The effective spring constant k_{eff} of the neck can be obtained from the slope of the force curve during the elastic stages. The variation of this spring constant for contact areas ranging from 1.2 to 6.9 nm^2 can be clearly seen in the different slopes of the force curve in Fig. 2. Figure 3(c) shows the k_{eff} values obtained from the force curve of Fig. 2(b). We use continuum contact mechanics to compute k_{eff} with the equation [16] $k_{\mathrm{eff}} = BEa/(1 - \nu^2)$, where a is the radius of the contact, ν is Poisson's ratio
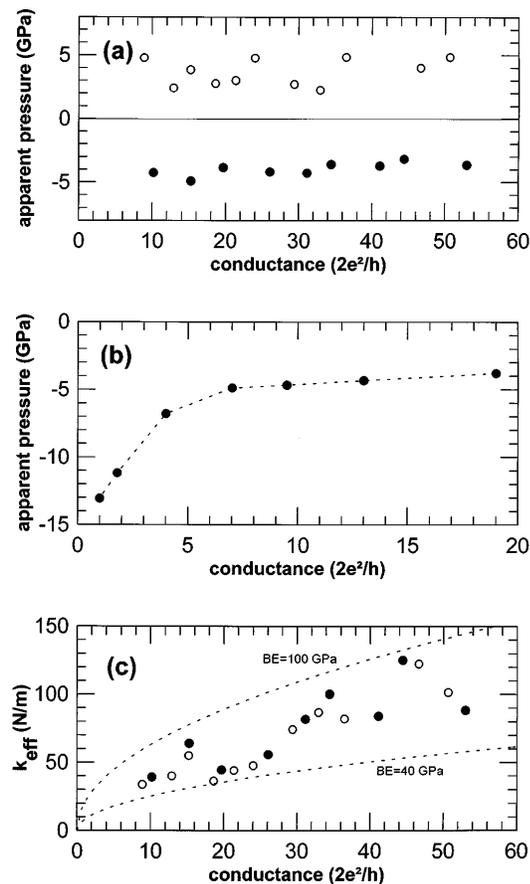
FIG. 3. (a) Plot of the maximum compressive (positive) and tensile (negative) apparent pressure (open circles and solid circles) before atomic rearrangements obtained from the force curve of Fig. 2. (b) The same computation of the minimum tensile apparent pressure is plotted here for the force curve in Fig. 1. (c) The effective spring constant k_{eff} of the constriction can be obtained from the slope of the elastic stages of the force curve considering an equivalent spring for the constriction, in series with the effective spring constant of the cantilever beam. Here k_{eff} is computed from the force curve of Fig. 2. The open circles correspond to the compressive branch of the cycle and the solid circles to the tensile branch of the force curve. The two dashed lines are the continuum mechanics computations considering limiting values of $BE = 40$ and 100 GPa.

(0.42 for Au), E is Young's modulus, and B is a factor that depends on the geometry of the contact. B can be considered to be between 1 and $2/3$ for these contact geometries. Young's modulus of gold ranges from 43 to 117 GPa depending on the crystalline direction. The two dashed lines in Fig. 3(c) are the continuum mechanics computations considering limiting values of $BE = 40$ and 100 GPa. This experiment shows that continuum contact mechanics can be applied to estimate the elastic properties of these types of nanostructures down to contact areas whose conductance is 10 quantum units. The small oscillation in the curves is due to the mechanical vibration of the cantilever beam. The frequency of this oscillation depends on the effective spring constant of the cantilever

beam in series with the effective spring constant of the constriction. The values of k_{eff} computed from the frequency of the oscillation are consistent with those measured from the slope of the elastic stages.

In several recent experiments the fact that the conductance shows abrupt steps has been taken as an indication of quantization [5,6]. Krans *et al.* [3] have pointed out recently that, in order to distinguish in the conductance measurements quantization effects from those of discrete variation in the contact size, other experimental information in addition to the abrupt steps in conductance must be considered. This point of view is supported by our experimental results that show for the first time that for gold contacts at room temperature the abrupt changes in conductance are *always* due to atomic rearrangements, and that atomic rearrangements *always* cause abrupt changes in the conductance.

In summary, in this Letter we report results on the mechanical properties of atomic-sized gold contacts at room temperature and their relation to electrical properties. We find that the force needed to break the smallest contact has a quite well defined value and possibly corresponds to one single atom. The elastic properties of these contacts can be estimated using continuum contact mechanics while their strength is much higher than for macroscopic contacts. We also show that the jumps in electrical conductance during the deformation of an atomic-sized neck are *always* correlated to mechanical force relaxations and consequently to atomic rearrangements.

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