Quantized Conductance of a Single Magnetic Atom

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A single Co atom adsorbed on Cu(111) or on ferromagnetic Co islands is contacted with non-magnetic W or ferromagnetic Ni tips in a scanning tunneling microscope. When the Co atom bridges two non-magnetic electrodes conductances of $2e^2/h$ are found. With two ferromagnetic electrodes a conductance of $e^2/h$ is observed which may indicate fully spin-polarized transport.

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The conductance of nanometer-sized contacts may be decomposed into contributions of transport eigenchannels according to $G = G_0 \sum_{i=1}^n \tau_i$, where $G_0 = 2e^2/h$ is the quantum of conductance (e: electron charge, h: Planck’s constant), and $\tau_i$ is the transmission probability of the $i$th channel [1, 2]. The factor 2 in the quantum of conductance is due to spin degeneracy. In contacts involving magnetic electrodes the spin degeneracy of transport channels may be lifted. Each spin-polarized channel then may contribute up to $G_0/2$ to the total conductance.

A quantized conductance of $G_0/2$ is expected when a fully spin-polarized current is transmitted with a probability of 1 through a spin-polarized transport channel. These conditions appear difficult to fulfill. Nevertheless, experimental observations of conductance quantization in units of $G_0/2$ have repeatedly been reported [3, 4, 5, 6, 7, 8]. These conductances were observed with [4, 6] or without [3, 5, 7, 8] external magnetic fields, for ferromagnetic [3, 4, 5, 6, 7] and non-magnetic electrodes [7, 8]. On the other hand, the absence of non-integer conductance quantization has also been inferred from experimental results [9, 10]. Untiedt et al. showed that contaminants like H$_2$ or CO modify the conductance and could, in the case of CO adsorption on Pt electrodes, give rise to a conductance of $G_0/2$ [10]. A considerable variety of model calculations [11, 12, 13, 14, 15] have been performed and support the notion that conductance quantization in units of $G_0/2$ is not expected from the investigated ferromagnetic contacts. It should be noted, however, that the modeling performed so far did not include geometrical relaxations of the contacts although the importance of the detailed atomic arrangement has been emphasized [11, 15, 16, 17].

The contradictory conclusions reached from the various experiments may be related to a lack of characterisation of the atomic details of the junction. This problem may be reduced by using a cryogenic scanning tunneling microscope to probe the conductance of clean single-atom contacts in ultra-high vacuum. Here we apply this approach to investigate prototypical junctions. A single magnetic atom on a spin-polarized island or a non-magnetic substrate is contacted with non-magnetic and ferromagnetic tips. We find that the conductance of a single Co atom is $G_0$ when two non-magnetic electrodes are used. With ferromagnetic electrodes the conductance is $G_0/2$. Conductances of $\approx 0.9 \times G_0$ are observed for a combination of a non-magnetic and a ferromagnetic electrode. In contrast to previous experiments, the contact geometry and chemistry are characterised by imaging of the contact area prior to and after conductance measurements. We hint that the observed conductance may be related to the detailed geometry and bonding at the contact.

The experiments were performed using a home-built scanning tunneling microscope operated at 7 K and in ultra-high vacuum with a base pressure of $10^{-9}$ Pa. The Cu(111) surface as well as chemically etched W and Ni tips were cleaned by argon ion bombardment and annealing. Tungsten and Ni tips were fabricated from 0.25 mm thick wire of 99.99% purity. Cobalt deposition onto Cu(111) was performed at room temperature using an electron beam evaporator and a Co evaporant of 99.99% purity. Single Co atoms were deposited onto the cold sample surface through openings in the cryostat shields. The tip magnetization direction is dictated by the shape anisotropy since magnetocrystalline anisotropy is small in Ni. Therefore, the tip is magnetized along its axis leading to a magnetization perpendicular to the substrate surface [18]. Cobalt islands on Cu(111) are well studied [19, 20, 21] and identified as single-domain ferromagnetic exhibiting a perpendicular magnetization with strong coercivity and remanence [21].

Figure 1 shows a pseudo-three-dimensional scanning tunneling microscopy (STM) image of a Co island and single Co atoms adsorbed on Cu(111) at 7 K. The Co island exhibits a triangular shape and a thickness of two Co layers as expected. On top of the island a single Co atom was adsorbed. These surface structures together with a non-magnetic W or a ferromagnetic Ni tip provide four contact configurations. The W or Ni tip may contact a Co atom adsorbed on the non-magnetic substrate surface or on a ferromagnetic Co island.

Cleanliness of the tip as well as of the Cu(111) surface and the surface of adsorbed Co islands was monitored by spectroscopy of the differential conductance (d$I$/d$V$). The Shockley-type surface state of Cu(111) was observed...
as a sharp step-like onset of $dI/dV$, while Co islands exhibited occupied as well as unoccupied $d$ states as pronounced peaks in spectra of $dI/dV$ [21]. Therefore, the presence of contaminants, in particular of hydrogen, adsorbed on the substrate or the islands can be safely ruled out. Moreover, hydrogen adsorbed on Co islands has recently been shown to desorb by using tunneling currents exceeding 20 nA [22]. In the contact experiments reported here, currents of the order of 10 $\mu$A are passed through the islands.

Figure 2 displays the conductance of a single Co atom between different combinations of electrodes, as a function of the displacement $\Delta z$ of the microscope tip. For small tip displacements the conductance varies exponentially with the displacement as expected for the tunneling regime (denoted 1 in Fig. 2). In a transition region (2) the conductance rapidly increases. Finally, a smaller variation of the conductance occurs in the contact region (3). To define a contact conductance, $G_c$, we approximate the conductance data in the transition and contact regions by straight lines. Their point of intersection defines the contact conductance. This definition has previously been used for contacts to noble metal atoms and molecules and was found to reproduce their expected contact conductances [23]. Conductance values obtained from Co atoms according to this procedure are summarized in Table 1.

While for the W – Co – Cu junction the contact conductance is $\approx G_0$, which is in agreement with single-Co conductance measured on Cu(100) [24], we observe lower contact conductances with ferromagnetic electrodes. The most striking result is obtained when a Co atom adsorbed to a Co island is contacted by a ferromagnetic tip. In this case the contact conductance is $\approx G_0/2$. Combinations of non-magnetic and ferromagnetic electrodes lead to Co atom conductances of 0.88 $G_0$ (W – Co – Co) and 0.85 $G_0$ (Ni – Co – Cu).

We note that conductance curves acquired for voltages $|V| \leq 0.1$ V exhibited the same characteristics as presented in Fig. 2. Voltages $|V| > 0.1$ V led to an enhanced

![FIG. 2: (Color online) Conductance $G$ vs. tip displacement $\Delta z$ recorded from a single Co atom with different electrode combinations. W or Ni tips are used to contact a single Co atom on a Cu substrate or on a Co island. Squares: W – Co – Cu, lozenges: W – Co – Co, triangles: Ni – Co – Cu, circles: Ni – Co – Co. Tunneling (1), transition (2) and contact (3) regions of the conductance curves are indicated. Linear fits to the data in the transition and contact regions are used to define a contact conductance $G_c$. $\Delta z = 0$ corresponds to $V = 100$ mV and $I = 500$ nA prior to opening the feedback loop of the microscope. The conductance curves for the W – Co – Cu, W – Co – Co, and Ni – Co – Cu contacts were vertically offset by 0.6 $G_0$, 0.4 $G_0$, and 0.2 $G_0$, respectively.]

![FIG. 1: (Color online) Pseudo-three-dimensional representation of a constant-current STM image of a triangular Co island adsorbed on Cu(111). Single Co atoms that are adsorbed on the substrate surface and on top of the island appear as protrusions (sample voltage: $V = 100$ mV, current: $I = 100$ pA, size: 24.5 nm × 24.5 nm).]
mobility of Co atoms adsorbed on Co islands. We experienced the Co atom to change its adsorption site - either to the tip or to an adjacent site on the island - during tip excursion toward the adsorbed atom.

These results clearly show that the conductance of a ferromagnetic Ni – Co – Co contact is close to $G_0/2$. At present, it is not clear whether this value is due to transport through a combination of partially open channels or, most excitingly, a single fully spin-polarized channel. In any event, the experimental result appears to contradict available modeling results for transport through magnetic atoms. It calls for calculations which take into account the detailed structure and bonding of the junction.

We suggest that relaxations of the atomic positions in the contact region may be at the origin of this discrepancy. Recent theoretical work by Häfner et al. lends support to this interpretation. The conductance of atomic-size Co and Ni contacts and the spin polarization of the current were reported to be very sensitive to the contact geometry. In particular, for electrode separations at contact, however, the spin polarization was predicted to drop sharply to zero over a range of $\approx 0.5\,\text{Å}$. Relaxations of atomic positions owing to adhesive forces, which have been found for other single-atom [25] and single-molecule [26] contacts, were not included in these calculations. They may shift the range of distances where spin polarization is lost. This scenario, which remains to be analyzed by detailed calculations, would imply that the observed $G_0/2$ conductance is due to a fully spin-polarized channel.

In conclusion, we observed a conductance of $G_0/2$ from single Co atoms between ferromagnetic electrodes. The contacted atom as well as the status of the electrodes were characterized by imaging and spectroscopy of the atom and the hosting surface. The observed conductance reduction from $\approx 1\,G_0$ to $\approx G_0/2$ appears to contradict available modeling results for transport through magnetic atoms. It calls for calculations which take into account the detailed structure and bonding of the junction.

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