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 nonmagnetic W or ferromagnetic Ni tips in a scanning tunneling microscope. When the Co atom bridges two nonmagnetic electrodes a conductance of $\approx 2e^2/h$ is found. With two ferromagnetic electrodes a conductance of $\approx e^2/h$ is observed.

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The conductance of nanometer-sized contacts may be decomposed into contributions of transport eigenchannels according to $G = G_0 \sum \tau_i$, where $G_0 = 2e^2/h$ is the quantum of conductance ($-e$: electron charge, h: Planck's constant), and τ_i is the transmission probability of the ith 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 [3–8]. These conductances were observed with [4,6] or without [3,5,7,8] external magnetic fields, for ferromagnetic [3–7] and nonmagnetic electrodes [7,8]. On the other hand, the absence of noninteger 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 [11–15] 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 [11,15–17].

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 can be reduced by using a cryogenic scanning tunneling microscope (STM) to probe the conductance of clean single-atom contacts in ultrahigh vacuum. Here we apply this approach to investigate prototypical junctions. A single magnetic atom on a ferromagnetic island or a nonmagnetic substrate is contacted with nonmagnetic and ferromagnetic tips. We find that the conductance of a single-Co atom is $\approx G_0$ when two nonmagnetic electrodes are used. With ferromagnetic electrodes the conductance is $\approx G_0/2$. Conductances of $\approx 0.9 G_0$ are observed for a combination of a nonmagnetic and a ferromagnetic electrode. In contrast to previous experiments, the contact geometry and chemistry are characterized 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 ultrahigh vacuum with a base pressure of 10^{-9} Pa. Tungsten and nickel tips were cut from 0.25 mm thick polycrystalline wire of 99.99% purity and then chemically etched in diluted NaOH and HCl, respectively. *In vacuo*, tips and Cu(111) surfaces were prepared by argon ion bombardment and annealing. Tungsten tips were further prepared by controlled tip-surface contacts, which most likely led to copper-covered tip apices. Prior to mounting the Ni tips to the cold microscope scanner they were placed close to a CoSm permanent magnet. A similar treatment of polycrystalline Ni tips was reported to give rise to a spin polarization of tunneling electrons of at least 30% [18], which further increases with increasing current [19]. Moreover, the magnetization of such tips is preferentially oriented along their long axes [20] owing to the shape anisotropy, which dominates the small magnetocrystalline anisotropy in Ni. Particular care was taken to maintain the Ni tip apices clean during measurements, since small amounts of contaminants are known to reduce the spin polarization of tunneling electrons considerably [18]. Cobalt deposition onto Cu(111) was performed at room temperature using an electron beam evaporator and a Co evaporant of 99.99% purity. The resulting cobalt islands on Cu(111) are well studied [21–23] and identified as single-domain ferromagnetic exhibiting a perpendicular magnetization with strong coercivity and remanence [23]. These islands exhibit two stackings, which are referred to as unfaulted and faulted with respect to the substrate stacking [21]. Single-Co atoms were subsequently deposited onto the cold sample surface through openings in the cryostat shields.

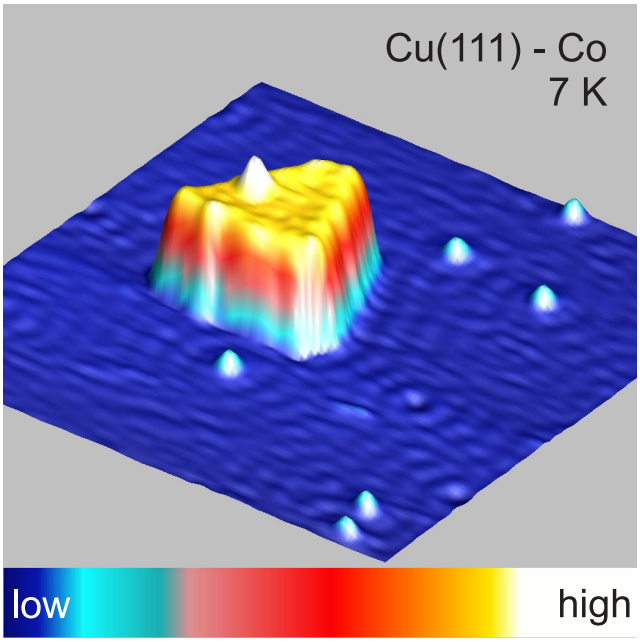

FIG. 1 (color online). Pseudo-three-dimensional representation of a constant-current STM image of a triangular Co island on Cu(111). Single Co atoms, which are adsorbed on the substrate surface and on top of the island, appear as protrusions. Sample voltage: $V = 100$ mV, current: $I = 100$ pA, size: 24.5 nm $\times$ 24.5 nm. The maximum apparent height is 4 Å at these parameters.

Figure 1 shows a pseudo-three-dimensional 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 is adsorbed. These surface structures together with a nonmagnetic copper-covered W or a ferromagnetic Ni tip provide four contact configurations. The W or Ni tip may contact a Co atom adsorbed on the nonmagnetic 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 (dI/dV). The Shockley-type surface state of Cu(111) was observed as a sharp steplike onset of dI/dV, while Co islands exhibited occupied as well as unoccupied d states as pronounced peaks in spectra of dI/dV [23]. Therefore, the presence of contaminants, in particular, of hydrogen, adsorbed on the substrate or the islands can be ruled out [24].

Figure 2 displays the conductance of a single-Co atom between different combinations of electrodes, as a function of the displacement Δz of the microscope tip [25]. For small tip displacements the conductance varies exponentially with the displacement as expected for the tunneling regime [denoted 1 in Fig. 2(a)]. In a transition region (2) the conductance rapidly increases. Finally, a smaller variation of the conductance occurs in the contact region (3). To

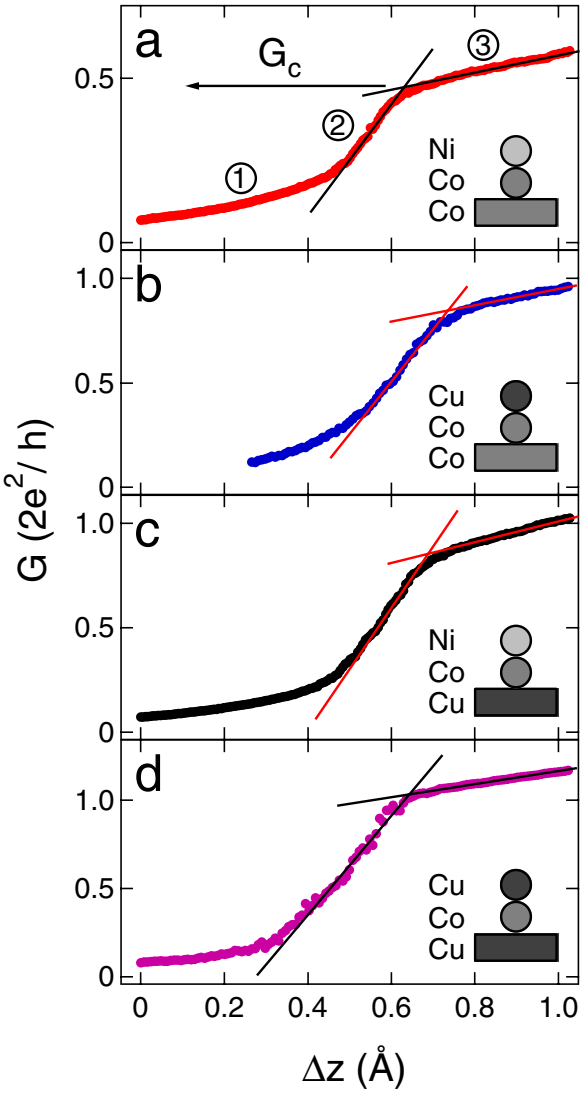

FIG. 2 (color online). Conductance G versus tip displacement Δz recorded from a single Co atom with different electrode combinations. (a) Ni–Co–Co. (b) Cu–Co–Co. (c) Ni–Co–Cu. (d) Cu–Co–Cu. Tunneling (1), transition (2) and contact (3) regions of the conductance curves are indicated in (a). Linear fits 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.

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 [26]. Conductance values obtained from Co atoms according to this procedure are summarized in Table I.

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 $\approx G_0/2$ [Fig. 2(a)].

TABLE I. Contact conductances G_c of a single Co atom for different electrode combinations. Uncertainty margins reflect the standard deviations of the contact conductances observed in repeated experiments.

Tip–Atom–Surface Materials	$G_c(G_0)$
Cu–Co–Cu	1.03 ± 0.02
Cu–Co–Co	0.88 ± 0.02
Ni–Co–Cu	0.85 ± 0.02
Ni–Co–Co	0.48 ± 0.02

Combinations of nonmagnetic and ferromagnetic electrodes lead to Co atom conductances of $\approx 0.88G_0$ [Cu–Co–Co, Fig. 2(b)] and $\approx 0.85G_0$ [Ni–Co–Cu, Fig. 2(c)]. The Cu–Co–Cu junction [Fig. 2(d)] exhibits the highest contact conductance of $\approx G_0$, which is in agreement with single-Co conductance measured on Cu(100) [27]. The contact conductance values of the Co atoms adsorbed on the Co islands do not depend on the stacking of the Co islands.

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 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. A systematic investigation of the conductance dependence on the Co atom adsorption site was hampered by this enhanced mobility. Nevertheless, we expect the Co atom to reside in a threefold coordinated hexagonal close-packed hollow site [28]. Moreover, all Co atoms, which were contacted in our experiments, were separated from island edges by more than 15 Å.

These experimental 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 this context Fig. 3 shows conductance curves for the Ni–Co–Co junction taken at positive (top) and negative (bottom) voltages. In both cases we observe a contact conductance of $\approx G_0/2$ indicating that this result is independent of the current direction through the junction. This observation is further indication that the ferromagnetic Ni tip and the ferromagnetic Co island act as sources and drains of spin-polarized electrons. The conductance traces in Fig. 3 were acquired one after the other without modifying the tip. We experienced that the shape of the conductance curve in the transition regime depends on the location on the adatom the tip is approached to. In the experiments the tip may be placed atop the center of the atom with an accuracy of ± 0.5 Å. Nevertheless, the conductance at contact remains unaffected. Preliminary calculations performed for Co atoms adsorbed on a double-layered Co film indicate that in contact with a Ni tip a spin-polarized

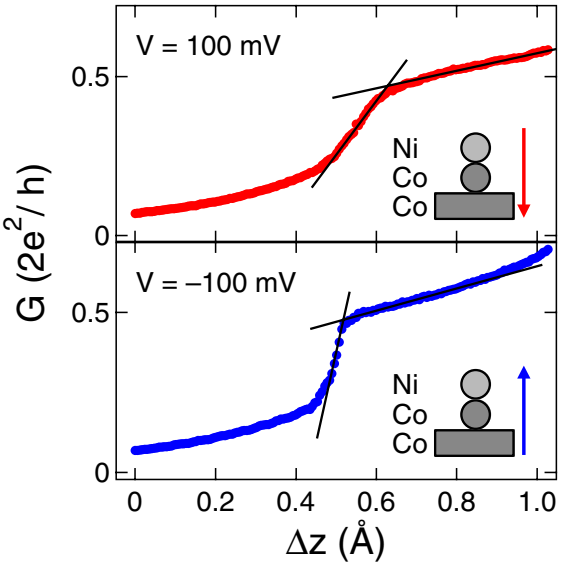

FIG. 3 (color online). Conductance traces for Ni–Co–Co junctions acquired at positive (top) and negative (bottom) sample voltages. The feedback loop was opened at 100 mV (top) or −100 mV (bottom) and 500 nA. Both conductance traces exhibit a contact conductance of $0.48G_0$. Insets: Sketches of the junctions with arrows indicating the directions of current flow.

transmission resonance exists around the Fermi level. This observation suggests that only electrons with a given spin polarization contribute to the current. In any event, the experimental result appears to contradict current modeling results on ballistic transport through magnetic constrictions which do not indicate conductance quantization in units of $G_0/2$. 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.* [15] 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 in the tunneling range, Häfner *et al.* calculated a conductance of essentially $G_0/2$ reflecting a spin polarization of the current of nearly 100%. For smaller electrode separations at contact, however, the spin polarization was predicted to drop sharply to zero over a range of ≈ 0.5 Å. Relaxations of atomic positions owing to adhesive forces, which have been found for other single-atom [29] and single-molecule [30] 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 $\approx G_0/2$ conductance is due to a fully spin-polarized channel.

In conclusion, we observed a conductance of $\approx G_0/2$ from single-Co atoms between ferromagnetic electrodes. The contacted atom as well as the state of the electrodes were characterized by imaging and spectroscopy of the atom and the substrate. The observed conductance reduc-

tion from $\approx 1G_0$ 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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