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Electronic picture of spin-polarized tunneling with a Cr tip

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ABSTRACT

We use spin-resolved scanning tunneling spectroscopy with a Cr-covered W-tip to investigate the magnetic switching of single Co islands on Cu(1 1 1) in polar magnetic fields. The observed hysteretic curve resembles a shape which is well known from so-called butterfly curves of tunneling magnetoresistance measurements. This indicates that not only the Co-island but also the Cr-tip changes its spin orientation in response to the applied magnetic field. For the interpretation of the experimental observations, we perform ab initio calculations by means of the Korringa–Kohn–Rostoker Green's function method. The calculations demonstrate that the Cr-tip is not a perfect antiferromagnet and has an uncompensated magnetic moment which changes its spin orientation continuously due to the applied magnetic field.

1. Introduction

Spin-resolved scanning tunneling microscopy (spin-STM) is a powerful tool to investigate magnetic properties on the atomic scale [1]. The relative spin orientation of the magnetic moments of sample and tip results in a spin contrast of the tunneling current. However, measurements of the contrast give no clear information about the individual change of the spin orientation of sample or tip in response to an external field, but only the relative change of spin orientation between tip and sample is measured. The individual spin orientation of both electrodes of the system, tip and sample, cannot be deduced a priori without preliminary model assumptions. In this respect the predictive role of first-principle calculations is of great importance. In previous publications the role of one electrode has been neglected based on the assumption that the tip [2,3] or the sample [4,5] has a fixed magnetization direction even under the influence of an external magnetic field.

In this paper we present a combination of experimental and theoretical investigations of the prototype system Co on Cu(1 1 1). Using spin-STM with a Cr-covered W-tip, we investigate the magnetic switching of single Co islands on Cu(1 1 1) by measuring a complete magnetic cycle of the differential conductance in fields of up to 4 T along the sample normal. The observed hysteretic curve resembles a shape that is well known from so-called butterfly curves of tunneling magnetoresistance measurements [6]. The result indicates that both Co island and Cr tip respond to the applied magnetic field. This observation is in contrast to the previously postulated picture of a fixed spin orientation of the Cr-tip.

For the interpretation of the experimental observations, we performed ab initio calculations based on the Korringa–Kohn–Rostoker (KKR) Green's function method. The calculations support the experimental observations and show that the conductance of the tunneling current changes smoothly with respect to the relative orientation between sample and tip magnetization.

2. Results

We investigate the magnetic field dependence of the differential conductance of Co on Cu(1 1 1). Previous studies showed that the easy axis of the Co islands is along the sample normal [2,7]. The Cu(1 1 1) substrate has been cleaned prior to Co deposition by cycles of ion bombardment (Ar^+, 1 keV, 1 μA) and subsequent annealing at 700 K. With deposition of submonolayer quantities of Co at room temperature, triangular double layer high island with a base length from a few nanometers up to 30 nm are formed [8,9] and subsequently characterized at 7 K by STM and scanning tunneling spectroscopy (STS). To obtain the differential conductance dI/dV, STS has been performed by a lock-in technique by applying an AC voltage (10 mV, 5 kHz) to the gap voltage [9]. The W-tip (electrochemically etched and subsequently flashed to 2400 K) is covered by Cr to obtain a spin contrast, where the Cr thickness was chosen in different experimental runs between 40 and 100 ± 10 monolayers (ML).

Fig. 1 shows a typically recorded differential conductance loop of a Co island during a cycle of the magnetic field. First we want to

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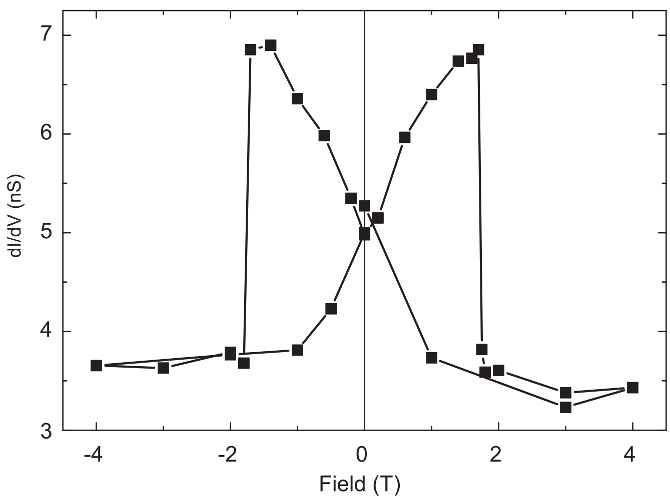

Fig. 1. Differential conductance loop of a Co island ($V_{gap} = -0.57$ V). The sharp drop at ± 1.75 T corresponds to the switching of the magnetization direction of the island.

point out the symmetric shape of the curve with respect to the field. We have performed several tip preparations with a Cr coverage between 40 and 100 monolayers and find consistently symmetric hysteresis cycles of the differential conductance. This shape of the curve is similar to butterfly curves of tunneling magnetoresistance measurements [6]. Secondly, the *dI/dV* signal shows a sinusoidal smooth shape with increasing field up to a critical field value of ± 1.75 T, where the signal changes abruptly. The measurements on different islands with the same tip apex show different critical field values, at which the signal has a sudden drop. This differences can be assigned to island properties (e.g. size, shape, and stacking sequence). On the other hand the sinusoidal behavior is unchanged. This observation indicates that not only the Co-island but also the Cr-tip changes its spin orientation in response to the applied magnetic field. The smooth behavior for small fields can be related to a continuous change of the spin orientation of the Cr-tip, while the sharp drop of the *dI/dV* signal has to be attributed to the sudden switching of the magnetization direction of the island.

In order to verify our statement, we performed ab initio calculations to study the influence of the relative spin orientation between tip and sample for different magnetic tip apex configurations. Our self-consistent calculations were done by means of the KKR Green's function method within the local spin-density approximation of the density functional theory [10] with an extension to non-collinear magnetism [11–14]. Ballistic conductance was calculated in the framework of the Landauer–Büttiker approach using KKR Green's functions including non-collinear magnetic order [12].

To simulate the experimental tunnel junction, we use two semi-infinite Cu(1 1 1) electrodes, one with a 2 ML Co coverage and one with a cluster of Cr atoms forming a tip on top, separated by a vacuum barrier of three equivalent Cu ML. A single atom or a tetrahedron consisting of four atoms were used as tips. For the tetrahedral tip we calculated all possible collinear spin configurations of the atomic magnetic moments. In Table 1 the local magnetic moments are presented. Atom 1 is always the last tip atom and atoms 2–4 are the base of the tetrahedron next to the surface. The coordination of atom 1 is lower than the one for the base atoms. This leads to an enhancement of the magnetic moment for atom 1 relative to the others. As a consequence, the total magnetization M_{Total} of the tip is non-zero for all configurations under consideration. This means that the Cr tip has a remaining total magnetization to interact with an external

Table 1
Local magnetic moments (in μ_B) of the Cr tip atoms in the tetrahedral configuration.

	FM	AFM1	AFM2	AFM3
Atom 1	4.63	4.43	4.49	4.56
Atom 2	4.21	−4.15	3.97	4.07
Atom 3	4.21	−4.15	−4.01	4.07
Atom 4	4.21	−4.15	−4.01	−3.91
M_{Total}	17.26	−8.02	0.45	8.80
$E-E_{FM}$ (mRy)	0.00	−48.10	−76.08	−60.24

M_{Total} is the sum over all moments and $E-E_{FM}$ is the total energy difference with respect to the ferromagnetic solution. Atom 1 is the front atom of the tip, while atoms 2–4 are forming the base of the tetrahedron on the substrate.

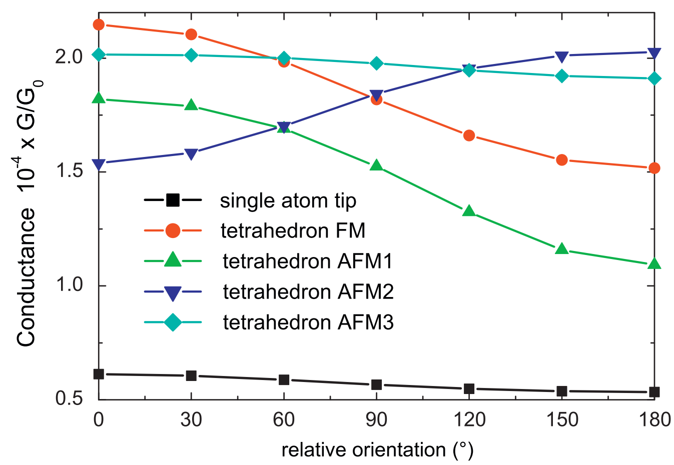

Fig. 2. Conductance as a function of the relative spin orientation between Co layer and Cr tip magnetization. The different curves are calculated for the single Cr atom tip and the tetrahedral tip assuming different spin configurations.

magnetic field. The total energy calculations show that the energetically favored configuration is the AFM2 configuration, where two atoms have magnetic moments pointing upwards and two atoms have magnetic moments pointing downwards. In the case of the single atom Cr-tip, the magnetic moment of the atom is 4.31μ_B. One could argue that the simulation of the tip by a small cluster of Cr atoms does not fit the experimental setup. Another assumption [15] based on the antiferromagnetism of bulk Cr claims that the spin orientation of the tip apex remains fixed, and the magnetization of the Co island could be either parallel or antiparallel to it. In fact, the tip in the experimental setup consists of at least 40 ML of Cr. However, even in this case the sharp front of the tip deviates from bulk behavior and causes different local magnetic moments of the apex Cr atoms in comparison to bulk. This difference causes uncompensated magnetic moments and results in a non-zero tip magnetization.

To study the influence of the different spin configurations at the Cr tip apex on the tunneling current, we calculated the conductance at zero bias in dependence on the relative orientation between Co and tip magnetization (Fig. 2). Independent of the specific spin configuration of the Cr tip, a sinusoidal behavior of the conductance with respect to the relative orientation between Co and Cr tip magnetization is observed. Different spin configurations and geometries change the absolute values of the conductance. The calculated results support the experimental observation and show that the conductance of the tunneling current changes smoothly with respect to the relative orientation of the magnetization. Comparing the calculated conductance curves (Fig. 2) with the measured *dI/dV* signal (Fig. 1) leads to the conclusion that the Cr-tip changes the spin orientation in response to the external magnetic field.

3. Conclusion

We present differential conductance measurements of single Co islands on Cu(1 1 1) by means of spin-resolved scanning tunneling microscopy with a Cr-covered W-tip. The observed hysteretic curve indicates that not only the Co-island but also the Cr-tip changes its spin orientation in response to an applied magnetic field. The influence of different spin configurations of the Cr tip apex on the conductance of the tunneling current is investigated theoretically. We find that uncompensated Cr spins are expected at the Cr tip apex. The calculated change of conductance as a function of the relative angle between tip and sample magnetization supports the experimental results.

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