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Influence of step edges and strain on the domain wall width

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The influence of substrate steps and epitaxial strain on magnetic domain walls in thin films was investigated by means of spin-polarized scanning tunneling spectroscopy (Sp-STS). Domain walls in a 2 ML Fe film grown on a W(001) substrate were imaged. The domain wall width is considerably reduced when the wall is located at the step edge. This is explained by the atomic arrangement at the step edges and their influence on the ferromagnetic exchange and magnetic anisotropy. Measurements of the width of domain walls in 4 ML Fe films indicate a reduced exchange constant compared to bulk Fe. This effect is related to the reduced dimensionality but also to the huge strain of 10% in the Fe films.

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Low-dimensional systems such as thin films, wires, dots, and small particles are the focus of current interest. The motivation for studying these systems is not only limited to the fundamental level but it is also strongly encouraged by possible applications, like the increase of density in magnetic storage.[1] One of the important problems in this field is the understanding of the magnetization reversal process involving the nucleation and propagation of magnetic domain walls.[2] In the case of domain wall displacement, different defects in the thin film can lead to the pinning of the walls. As a consequence, the reversal process may be slowed down or even stopped. The understanding on the fundamental level of the influence of defects (step edges,[3] constrictions,[4] etc.) on the magnetic domain walls is therefore of great importance. Recent studies have shown that a high density of step edges can lead to highly anisotropic domain wall propagation.[3] Direct observation of the domain walls pinned at the step edges was, however, not possible up to now. Recently, Pietzsch *et al.*[5] observed domain walls in Fe thin films on W(110) and showed that the wall width is drastically reduced when pinned at structural constrictions, in agreement with theory.[4] Direct investigation of the domain wall in this case was possible by using spin-polarized scanning tunneling spectroscopy (Sp-STS) (Ref. 6).

Here we report on an Sp-STS study of thin Fe films on W(001). We directly observed free walls and walls pinned at step edges of the substrate. We show that the domain wall width is drastically reduced when pinned at step edges similar to the case of structural constrictions. As the wall energetics is governed by the relevant micromagnetic energies (the magnetic exchange, the magnetic anisotropy, and the magnetic stray field), the observed wall widths contain valuable information on these microscopic parameters. For the pinned walls, a reduction of exchange and an increase of anisotropy is suggested. In fully strained 4 ML Fe films on W(001), we found a reduced wall width which we relate partly to finite-size effects and to a the large biaxial strain decreasing the overlap.

All experiments were performed in ultrahigh vacuum (UHV) at a base pressure of 5×10^{-11} mbar. The W(001) crystal was cleaned by cycles of heating in oxygen and subsequent flashing to 2500 K. The cleanliness of the sample was checked by Auger electron spectroscopy (AES), low electron diffraction (LEED), and scanning electron microscopy (STM). Fe (99.999%) was deposited on the clean W(001) substrate by molecular beam epitaxy. After growth, the samples were characterized structurally and chemically by AES, LEED, and STM. For the STS and Sp-STS measurements we used a modified commercial cryogenic STM system. The spectroscopic data were obtain by a modulation of the gap voltage (U_{mod}=30 mV) and by detecting the differential conductivity dI/dV by a lock-in technique. We used etched W tips, flashed in UHV, coated with 10–15 ML of Fe, and followed by a short annealing, as described by Bode *et al.*[7] The Fe-coated tips are known to be sensitive to an in-plane component of the magnetization.[7] All our STS and Sp-STS measurements were performed at about 25 K.

In previous studies, we investigated the growth and magnetism of ultrathin Fe films on W(001). In spite of the large misfit of 10.4% between Fe and W, Fe grows pseudomorphically up to 4 ML coverage when deposited at temperatures between 400 and 500 K (Refs. 8 and 9). At 500 K and for Fe coverages above 5 ML, cross-shaped islands are nucleated on a 2 ML carpet of pseudomorphic Fe [see, for example, Fig. 2(d)]. The cross-shaped islands are relaxed via dislocations parallel to the ⟨100⟩ directions. Magnetic measurements[8,9] showed that the islands are magnetized in plane, with ⟨100⟩ directions as easy axis. Films up to 4 ML are pseudomorphic and are in-plane magnetized, but show a fourfold magnetic anisotropy with easy axis along the ⟨110⟩ directions. Details about the growth and the magnetic properties of Fe thin films grown on W(001) can be found in (Refs. 8 and 9).

As a first step towards magnetic Sp-STS studies the local density of states of Fe structures of different thickness was investigated. Averaged spectra of the differential conductivity dI/dV taken above pseudomorphic 2, 3, and 4 ML films and thicker cross-shaped islands (≈10 ML thick) are shown in Fig. 1(a). The empty-state peak at 0.25 V measured on the thicker islands corresponds nicely to the well-known surface state of bulk Fe(100) (Refs. 10 and 11). The spectra taken above the 3 and 4 ML islands show an empty-state peak and a shoulder at about 0.35 V. In addition, for the 4 ML islands, a filled-state peak is slightly visible at −0.25 V. The spectrum taken above the 2 ML Fe film is different. It shows a

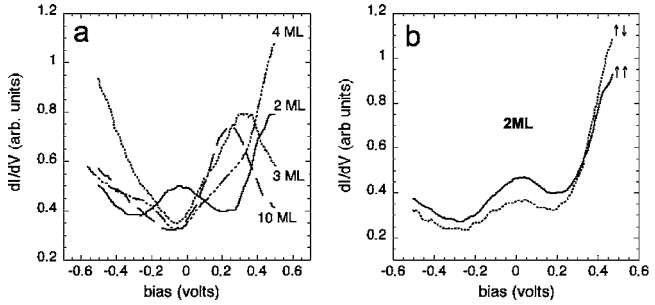

FIG. 1. (a) Averaged dI/dV spectra taken above pseudomorphic 2, 3, and 4 ML films and thicker cross-shaped islands ($\approx$10 ML thick). (b) Averaged spectra of dI/dV taken with a magnetic Fe-coated tip above two differently oriented magnetic domains on the 2 ML Fe film on the W(001) substrate.

filled-state peak at about −0.1 V. The peak position does not vary but the peak intensity is a function of relative magnetic orientation between tip and sample magnetization. We used these specific electronic states to obtain magnetic contrast by means of Sp-STS.

We focus on domain walls in 2 ML thick Fe films. The topographic image of a 2.3 ML thick Fe film grown on the W substrate at about 400 K is shown in Fig. 2(a). On top of a continuous 2 ML thick carpet of Fe, 3rd ML islands are nucleated and are visible as white dots. The spatially resolved differential conductivity dI/dV of the same area, simultaneously measured with an Fe covered tip at a bias of 0.3 V, is shown in the Fig. 2(b). Contrasts of different origin are observed in the dI/dV image. First, a thickness-related contrast can be seen between the 2 ML film and the 3-ML high islands. This contrast is due to the different electronic structure: the dI/dV at 0.3 V for the 3-ML areas is higher than that of 2 ML [see Fig. 1(a)]. Therefore, the 3 ML islands appear brighter. An additional contrast of magnetic origin is observed on the 2 ML Fe film. Magneto-optical Kerr (MOKE) measurements showed that the 2 ML Fe film is paramagnetic at room temperature.[8,9] When the temperature is reduced below 260 K, the 2 ML film becomes ferromagnetic[12] and magnetic domains are formed in the film. Two magnetic domains, separated by a domain wall, can be observed as "intermediate" and "dark" regions in the Fig. 2(b). The domain wall is pinned between the 3 ML thick islands. Averaged spectra of dI/dV taken above two different oriented magnetic domains are shown in the Fig. 1(b). The shape of the two spectra is similar with identical peak position, but the intensities of the peaks are different indicating that the two regions have identical electronic structures, but different spin populations. This shows that the intermediate and the dark regions on the 2 ML Fe film are related to differently magnetized areas with different projections with respect to the tip magnetization (close to the parallel and antiparallel configuration indicated by a maximum in contrast).

This magnetic contrast was found regularly. Typically, at least three contrast levels were resolved in agreement with the fourfold anisotropy. The rotation angle of the wall can be determined from the contrast change. A line profile (averaged over eight scan lines in the white box) taken across a 90° domain wall separating two magnetic domains is depicted in Fig. 2(c). The filled circles represent the experimental data and the continuous line is a fit with a standard wall profile: $\tanh(2x/w)$. As a result of this fit, the domain wall width was found to be: $w=12.4\pm2.2$ nm. This value is by a factor of 2 smaller than the 90° domain wall width in bulk Fe (Ref. 13) and a factor of about 20 smaller than the surface domain wall width on Fe whiskers.[14]

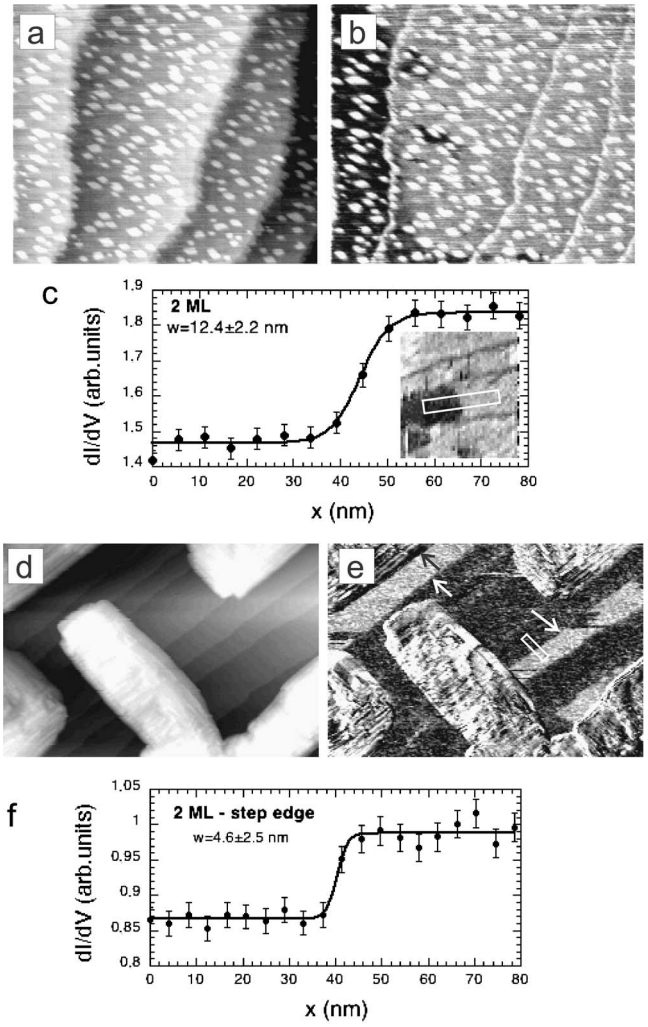

FIG. 2. (a) Topography of 2.3 ML Fe grown on W(001) at 400 K. (b) Map of the differential conductivity dI/dV of the same region at 0.3 V. The size of the two images is 535×458 nm. (c) Averaged line profile taken across a 90° domain wall. The filled circles represent the experimental data and the continuous line is a fit with a standard wall profile $\tanh(2x/w)$. (d) Topography of nominally 6 ML Fe grown on W(001) at 500 K. (e) Map of the differential conductivity dI/dV of the same region at 0.3 V. The size of the two images is 745×505 nm. (f) Line profile across the 90° domain wall pinned at the step edge. The filled circles represent the experimental data and the continuous line is a fit.

To understand the reduced wall widths, we focus on the energetics of domain walls in thin film. While in bulk Fe, Bloch walls are energetically favored, the stray field energy of the core of this type of wall is not negligible in thin films. Below a critical thickness in the range of the Bloch wall

width, Bloch walls become unstable and the more favorable Néel walls are observed.[13] In these walls, the magnetization rotates in the film plane. In the limit of ultrathin films (thickness $d \ll w$), "the wall width w is mainly determined by the exchange constant A and the anisotropy K but not the stray field energy."[15] For a 180° bulk Bloch domain wall, the width w is given by $w=2\sqrt{A/K}$ (and for a 90° it is half of this). In the ultrathin limit, the Néel wall width is given by the same expression,[15] which allows a comparison of the microscopic parameters of bulk and ultrathin systems. This is a consequence of the vanishing stray field in bulk Bloch walls (walls are charge free) and the negligible stray field in Néel walls in the ultrathin limit due to the large aspect ratio w/d of the wall (or alternatively the vanishing demagnetization factor N of the extremely flat core of the wall).

The reduced wall width in 2 ML Fe on W(100) compared to bulk Fe is due to two reasons. First of all, the anisotropy in both systems differs. For bulk Fe, an anisotropy of $K=5.4\times10^4$ J/m^3 has been reported,[16] while we estimate an anisotropy of $\approx -1.6\times10^5$ J/m^3 from measured surface and bulk contributions of the anisotropy in Fe/W(001) (Ref. 17). Secondly, the exchange constant A in 2 ML Fe is strongly reduced. As the atoms in the bcc (100) plane are not nearest neighbors but only next-nearest neighbors, the finite thickness of the film reduces the number of magnetic nearest neighbors by a factor of 2 compared to bulk Fe. It is known that the mesoscopic exchange constant A scales with the number of nearest and less strongly with the next-nearest neighbors of an Fe atom.[18] As a consequence, the exchange constant A decreases for 2 ML thick films. Both effects together explain the narrow walls in 2 ML films, satisfactory.

The domain wall width, however, can be influenced further by the local film structure. In some particular cases, domain walls were pinned by W substrate step edges. Figure 2(d) shows a topographic image of an annealed film. The large islands are about 10 ML high, being relaxed via dislocations parallel to the ⟨100⟩ directions. Between the islands the W substrate is covered by a fully strained and continuous 2 ML thick Fe film. The film covers also the substrate W steps, which are visible as long and straight lines in the image. Figure 2(e) shows the local dI/dV signal of the same area. Again, the contrast seen in the dI/dV image between the 10 ML islands and the 2-ML Fe film is due to their difference in electronic structure [see Fig. 1(a)]. On the 2 ML film, contrast of magnetic origin is observed. Several magnetic domains separated by 90° domain walls can be seen, some of them being pinned at the step edges [indicated by arrows in Fig. 2(e)]. A line profile (averaged over five scan lines in the white box) taken across one of the pinned domain walls is shown in the Fig. 2(f). In this case, the domain wall width was found to be $w=4.6\pm2.5$ nm, which is almost three times smaller than in the case of nonpinned domain walls [see Fig. 2(c)].

This further reduction of the wall width can be explained, when we take into account that the number of neighbors at the step edge of a 2 ML Fe film on W(100) is reduced. Depending on the local arrangement, two next-nearest neighbors in the bcc (100) plane (one at the top atomic layer of the upper step and one at the lower atomic layer of the lower step) and two nearest neighbors between different atomic

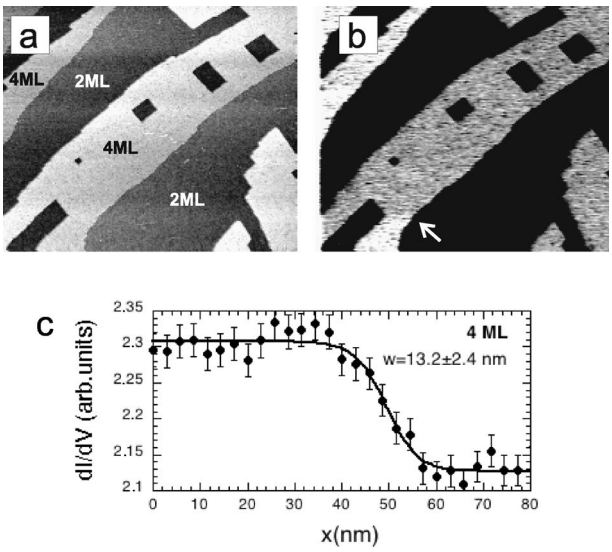

FIG. 3. (a) Topography of about 3 ML Fe grown on W(001) at 500 K ($U_{bias}=0.5$ V). (b) Map of the differential conductivity dI/dV of the same region at 0.5 V. The size of the two images is 755×358 nm. (c) Averaged line profile taken across the 180° wall indicated by an arrow in (b). The filled circles represent the experimental data and the continuous line is a fit.

planes (both in the atomic layer that runs continuously across the step edge) are missing at the step edge position. This reduces the exchange constant A and by this narrows the domain wall. Further, the step edges induce a large magnetic anisotropy[19,20] localized at the step edge. This increased anisotropy also may narrow the domain wall. Most likely both effects are operating leading to the large observed decrease of the wall width. This explains not only the narrowing of the wall but also the pinning mechanism. If the wall is positioned above a step edge the exchange energy is reduced.

Magnetic domains have also been investigated on 4 ML Fe films pseudomorphically grown on the W substrate. For the investigation about 3 ML of Fe were deposited at $\approx$ 500 K. At this temperature, 4 ML stripes are growing along the step edges while the rest of the film is 2 ML thick [Fig. 3(a)]. The spatially resolved differential conductivity dI/dV [Fig. 3(b)] was measured at 0.5 V simultaneously with the topographic image of the same area. As before, a thickness-related contrast is observed between the regions where the Fe film is 2 and 4 ML high, due to their different electronic structure [see Fig. 1(a)]. The dI/dV at 0.5 V for the 4 ML one is higher than the dI/dV at the same voltage for the 2 ML. Therefore, the 4 ML regions appear brighter than the 2 ML ones. The additional contrast observed between the 4 ML high stripes is of magnetic origin. The brighter 4 ML regions (upper left two stripes) are most probably magnetized parallel to the tip and the less bright ones (lower right stripes) are magnetized antiparallel to the same tip.

The contrast observed on the central stripe is also of magnetic origin. The domain wall (indicated by an arrow) is a 180 ° wall[23] and the line profile (averaged over four scan lines) taken across the wall is shown in Fig. 3(c). A fit was performed and the width of the domain wall was found to be

$w=13.2\pm2.4$ nm. The wall width can be related to the anisotropy constant K and the exchange constant A by using the expression $w=2\sqrt{A/K}$. We have determined the anisotropy constant K using hard axis loops measured with magneto-optical Kerr effect (MOKE): $K=44$ kJ/m^3 (Ref. 8). With this value, the exchange constant A for 4 ML films can be estimated to 2×10^{-12} J/m, which is about five times smaller than the bulk value $A=1\times10^{-11}$ J/m (Ref. 21). A similarly reduced value was also found in the case of 1 ML Fe on W(110) (Ref. 6), while for 2 ML Fe films on W(110) A was found to be 9×10^{-12} J/m, which is almost equal to the bulk value.[5] The smaller A in the case of 1 ML Fe on W(110) was explained by a reduced number of nearest neighbors and to the interaction with the nonmagnetic substrate. For 4 ML Fe film on a W(001) substrate we deduced an exchange constant five times smaller than the bulk value, which is rather surprising. In the 4 ML films, the averaged number of nearest neighbors is only reduced to 75% of the bulk value. Therefore, the low thickness is only partly responsible for the strong reduction. An additional reduction of the exchange constant A can, however, be caused by the immense strain in the Fe film. Due to its pseudomorphic growth, the in-plane lattice constant is stretched by $\approx10\%$. Taking into account that the atomic exchange J varies approximately as d^{-5}, where d is the interatomic distance,[22] the large strain in Fe almost halves the next-nearest neighbors exchange in the film plane giving a strong contribution to the reduced exchange constant A compared to the bulk value. Other effects, like a slight increase of the magnetic moment upon stretching of the lattice or variations of the magnetic anisotropy due to cooling the sample to 25 K are in the range of only 10% and by this may only cause changes of the wall with of the order of 5%.

In conclusion, we investigated magnetic domain walls on 2 and 4 ML Fe thin films pseudomorphically grown on a W(001) substrate. By measuring the domain wall width on the 2 ML film we could confirm for that the pinning of the domain wall at a step edge leads to the reduction of the domain wall width, similar to the case of domain walls pinned by structural constrictions. By using the domain wall width measured on the 4 ML Fe film together with *in situ* measurements of the magnetic anisotropy K, we could estimate the exchange constant A. We found that A is drastically reduced with respect to the bulk value most likely due to the reduced number of nearest neighbors and the strong strain in the film.

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[23] The wall runs along the ⟨110⟩ direction. The easy directions of magnetization are ⟨110⟩ (Ref. 9). This implies that 180° domain walls run along ⟨110⟩.