# Topological Frustrations in Mn Films on Fe(001)

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KEY WORDS Fe(001); Mn film; Sp-STM

ABSTRACT The high lateral resolution of spin-polarized scanning tunneling microscopy allows new insights into the spin structure of antiferromagnets on the nanometer range. We demonstrate the capability to image a well-defined in-plane component of the sample spin polarization and discuss the spin structure of antiferromagnetic bct Mn in contact with the ferromagnetic Fe(001) substrate. Mn atoms couple ferromagnetically within a Mn atomic plane, while normal to the surface a layer-wise antiferromagnetic order was found. Magnetic frustrations arise in this system at Fe substrate steps at the interface, where topologically induced 180° domain walls are created in the Mn film. A clear widening of the enforced domain walls with increasing Mn thickness was found. The measured widths could be fitted with a linear function and are explained on the basis of a Heisenberg model. *Microsc. Res. Tech. 66: 105–116, 2005.*  $_{0.2005 \text{ Wiley-Liss, Inc.}}$ 

## **INTRODUCTION**

The exchange coupling across the interface between ferromagnets and antiferromagnets (Meiklejohn and Bean, 1956) is of high importance for current applications in the field of magnetic storage. The interaction between the magnetic moments of the antiferromagnet and the ferromagnet is at the heart of exchange bias. In spite of the frequent use of this effect, the fundamental mechanisms occurring at the interface remain unknown to a large extent. As a model system, we studied the uncompensated, layer-wise antiferromagnet Mn in contact with the ferromagnet Fe. In principle, complex effects can occur caused by the exchange interaction at the interface in combination with defects. The most common structural defects are monatomic steps. When a layer-wise antiferromagnetic film overgrows a monatomic step of a ferromagnetic substrate, a difference in the thickness of one atomic layer between both sides of the step edge is created in the film. In the case of collinear coupling between the antiferromagnet and the ferromagnet, it is not possible to keep the ferromagnetic order in the ferromagnet, the antiferromagnetic order in the antiferromagnet, and the same magnetic coupling across the interface on both sides of the step edge. This conflict in the magnetic order leads to magnetic frustrations. Three possible configurations of magnetic frustrations have been proposed (Berger and Hopster, 1994; Berger and Fullerton, 1997; Morosov and Sigov, 2004). Either the antiferromagnet or the ferromagnet can be split into two domains separated by a frustration similar to a domain wall. The frustration starts at the step edge and extends into the antiferromagnet or the ferromagnet. Alternatively, a magnetic defect line is formed along the interface connecting two frustrations at interfacial steps. The region of magnetic frustration caused by such defects is often described as a domain wall. Close to the topological defect, the magnetically frustrated region cannot be described by a competition between the exchange and the anisotropy energy as in the case of conventional domain walls in ferromagnets or antiferromagnets. The magnetic frustration is pinned at the topological perturbation. The focus of this work lies on the investigation of magnetic frustrations in the model system of Mn on Fe(001) and their evolution with film thickness. The material system Mn/Fe(001) and the sample preparation are discussed in the following section. Here, spin-polarized scanning tunneling microscopy (Sp-STM) is used to investigate the local magnetic structure at the sample surfaces.

#### MATERIALS AND METHODS

Bulk Mn exists in a wide range of crystallographic structures. Up to 1,000 K, bulk Mn appears in a complex cubic phase  $(\alpha$ -Mn) with 58 atoms per unit cell and is antiferromagnetic below 95 K with a non-collinear spin arrangement (Shull and Wilkinson, 1953). Between 1,000 and 1,370 K, the cubic  $\beta$ -Mn is stable with 20 atoms per cell. A face-centered cubic  $(\gamma$ -Mn) and body-centered cubic  $(\delta$ -Mn) structure is found between 1,370 and 1,410 K and 1,410 K and the melting point, respectively (Wyckoff, 1963). Because of the simple atomic structure of the high-temperature phases ( $\gamma$  and  $\delta$  Mn), they have attracted attention in recent years. Mn can be stabilized at room temperature in a body-centered tetragonal (bct) structure on the (001) face of bcc Fe (Heinrich et al., 1987). Several groups confirmed the bct structure of Mn in this system up to about 20 ML (Andrieu et al., 1998a; Kim et al., 1996; Purcell et al., 1992). Low-energy electron diffraction (LEED) images and reflection high-energy electron diffraction (RHEED) oscillations recorded during the growth of Mn showed that Mn grows in a layerby-layer mode up to 10 to 25 ML (Tulchinsky et al., 2000). Indications of some defects and disorder were

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found (Pfandzelter et al., 1997; Pierce et al., 2000; Yamada et al., 2002) before the transition to threedimensional growth. The critical thickness strongly depends on the substrate quality, cleanliness, growth temperature, and rate. For substrate temperatures between 420 and 470 K, Tulchinsky and coworkers (2000) showed that the transition to three-dimensional growth takes place between 15 and 23 ML. Away from these growth conditions, the transition occurs at a lower thickness. The onset of three-dimensional growth is visible in the LEED pattern, where the intensity of diffraction spots fades away and a more complex diffraction pattern is observed. Additionally, RHEED oscillations vanish for the three-dimensional growth (Tulchinsky et al., 2000). Andrieu and coworkers (1998a) found that the RHEED pattern taken above the critical thickness is the same as observed on thick  $\alpha$ -Mn films on Ir(001). Thus, it is believed that thick Mn films deposited on Fe(001) relax in the  $\alpha$ -Mn structure. This behavior is characteristic for the Stranski-Krastanov growth mode of Mn-films. Thin Mn films grow pseudomorphically on Fe(001) with an out-ofplane lattice constant of 0.323 nm. However, a structural change was found between the second and third ML of Mn, which is interpreted as a modification of the out-of-plane lattice constant. The out-of-plane lattice constant increases after deposition of the second ML Mn (Andrieu et al., 1998a). When Mn was deposited at room temperature on Fe(001), no intermixing was found. The onset of intermixing was observed by Auger electron spectroscopy (AES) for substrate temperatures above 420 K (Andrieu et al., 1998a; Walker and Hopster, 1993). In STM studies, interdiffusion of Fe into the first ML Mn was found at substrate temperatures above 370 K (Bischoff et al., 2002). The intermixing was observed until the fourth Mn layer (Yamada et al., 2002). At the Mn surface of films between 4 to 10 ML, small regions with rectangular cross-shaped patterns start to form (Pierce et al., 2000; Yamada et al., 2002). It was speculated that these small rectangular islands are local reconstructions and a precursor to three-dimensional growth.

The first evidence that Mn on Fe(001) is a layer-wise antiferromagnet was presented by Walker and Hopster (1993). More recently, this was confirmed with scanning electron microscopy with polarization analysis (SEMPA) (Tulchinsky et al., 2000). There, only a spin polarization parallel to the Fe moment was found. The absence of an in-plane polarization perpendicular to the Fe magnetization was ascribed to two reasons. Either Mn couples solely collinearly to the magnetization of the underlying Fe substrate or non-collinear coupling is present but only in small domains below the resolution of SEMPA. Contradicting results exist concerning the magnetic coupling of the first and second Mn layer on Fe(001). Some groups confirm a ferromagnetic alignment of the magnetic moments of the first Mn layer (Andrieu et al., 1997a,b), whereas others found hints for an antiferromagnetic alignment (Rader et al., 1997; Roth et al., 1995). The investigation of the magnetic structure performed with SEMPA (Tulchinsky et al., 2000) suggests that the magnetic orientation of the first few layers is sensitive to the quality and crystallographic nature of the underlying Fe. Andrieu and coworkers (1998b) found that the sign of the coupling of the first Mn layer also depends on the amount of O on the substrate. The following discussion of Sp-STM measurements performed on Mn films on Fe(001) will be similar in case of ferromagnetic or antiferromagnetic coupling between the first Mn layer and the Fe substrate. No qualitative differences occur.

Sample preparation was carried out in ultra-high vacuum with a base pressure of  $1 \times 10^{-10}$  mbar. Before each measurement, the Fe-whisker was cleaned by Arsputtering and annealed to 900 K. No contamination could be found within the sensitivity of our AES. Mn was deposited at a substrate temperature of 370 K and the growth rate was determined by the monolayer period oscillations obtained by medium energy electron diffraction (MEED). The Mn coverage was derived from the analysis of MEED data. To increase the accuracy to fractions of a ML even in thicker films, STM images of the topography were used. STM images yielded a quite exact determination of the coverage between n and n + 1 ML. Thus, the integer coverage n was defined by MEED and the fractional coverage by topographic STM images.

After preparation, the samples were studied with Sp-STM at room temperature. In Sp-STM measurements, the spin-dependent tunneling current is used to investigate the spin polarization of a sample surface in addition to the topography. The spin polarization gives information of the local magnetization of a sample surface. In our Sp-STM, the non-magnetic tip is replaced by a ferromagnetic STM electrode (Wulfhekel and Kirschner, 1999). In this configuration, the tunneling current depends not only on the tip-sample distance, but also on their relative direction of spin-polarization as experimentally shown by Jullière (1975) and later explained theoretically by Slonczewski (1989). The spin-dependent tunneling current I is given by:

$$I = I_0 (1 + P_s P_t \cos \Theta), \tag{1}$$

where  $I_0$  presents the tunneling current without spin polarization of the electrodes,  $P_{s,t}$  is the spin polarization of the sample and the STM electrode, and  $\Theta$  is the angle between the directions of spin polarization of both. In our Sp-STM, the magnetization of the ring is periodically reversed with a frequency above the cutoff frequency of the feedback loop of the STM. The reversal corresponds to a change of theta by  $\pi$  and reverses the sign. Therefore, the feedback circuit that collects information on the sample topography sees only the average tunneling current  $I_0$  that does not contain spin information. With a phase-sensitive lockin amplifier, only the alternating part of the tunneling current  $\Delta I$  is detected, which is proportional to:  $P_s P_t$  $\cos\Theta$ , i.e., it contains all the spin information. This way, topographic and spin information are separated and an image of one spin component along the magnetization axis of the electrode can be recorded simultaneous to the topography (Wulfhekel and Kirschner, 1999). In our experiment, the magnetization of a ferromagnetic electrode is switched by applying a small alternating current to a coil wound around the electrode. This is schematically shown in Figure 1. The alternating magnetic field induced within the coil is large enough to fully reverse the magnetization of the



Fig. 1. Schematic representation of Sp-STM electrodes for measuring the in-plane component. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

ring-shaped electrode. In the ring electrode, the magnetization direction lies always tangential to the outer perimeter of the ring. Thus, at the bottom of the ring where the tunneling occurs, the magnetization lies in the plane of the sample surface. Because the magnetic flux in an ideal ring is closed, the magnetic stray field is zero. By choosing the plane in which the ring is oriented, the magnetization direction of the ring is defined and thus the direction of the sensitivity in the surface plane for the measured spin signal is known. One may wonder if such macroscopic rings used as an STM electrode do not significantly decrease the lateral resolution. As will be shown, the rings are not perfectly smooth and nano tips exist at the apex, which give a high lateral resolution. More details on the experimental setup can be found elsewhere (Schlickum et al., 2003).

#### RESULTS

As discussed above, Mn is a layer-wise antiferromagnet when grown on Fe(001) with in-plane spin polarization. Figure 2a shows a schematic model of the topographic and magnetic behavior of Mn layers on Fe(001). In the schema, ferromagnetic coupling between the first Mn layer and the Fe substrate was assumed, but antiferromagnetic coupling would not change the following results except the sign of the spin polarization. When several Mn layers are exposed at the surface, their magnetization points into an opposite direction on adjacent Mn terraces due to the layer-wise antiferromagnetic coupling. In Figure 2b and c, the topography and the corresponding spin signal taken with the Sp-STM on a 11.9 ML Mn film on Fe(001) are presented. Three different Mn layers are exposed at the surface, a nearly closed layer with some rounded holes and islands (see Fig. 2b). The Fe substrate was homogenously magnetized in one direction over the whole imaged area, as

determined by Kerr-microscopy. The direction of sensitivity of the ring was chosen collinear to the magnetization of the Fe substrate. Thus, the imaged spin signal shows the projection of the spin component collinear to the Fe magnetization. In the spin signal (Fig. 2c), the layer-wise antiferromagnetic order between the three different Mn layers is clearly visible. The spin polarization between adjacent Mn terraces is opposite, indicated by the black and white areas. The spin signal for *n* and n + 2 ML Mn is the same. This observation is in agreement with results found by Yamada and coworkers (2003). The Sp-STM measurement was performed with a bias voltage of 0.1 V at an average tunneling current of 3 nA. Under these conditions, the highest spin contrast was found. All following Sp-STM images were taken under these conditions. The spin contrast between oppositely spin-polarized Mn layers is about 1.2%. In spite of this low contrast, the signalto-noise ratio is high.<sup>1</sup>

The unperturbed layer-wise antiferromagnetic order is disturbed in case a step of the underlaying Fe substrate is present. Figure 3a sketches the topological and magnetic situation of Mn layers overgrowing a step edge of the Fe substrate underneath. The thickness of the Mn layers on both sides of a monatomic Fe step differs by one ML. This means n layers Mn are grown on the upper side of the Fe substrate step edge and n + 1 layers on the lower side. Due to the vertical lattice mismatch, subatomic steps are formed at the Mn film surface at the position of Fe step edges. The situation of the magnetic order above such step edges is more complicated. An undisturbed layer-wise antiferromagnetic coupling within the Mn film is not possible when the Mn moments at the interface on both sides of the step edge are aligned in the same direction by the Fe substrate. Instead, Mn layers that meet at the position of the Fe step edge have an opposite spin polarization. This leads to a magnetic frustration. When the Mn film thickness is smaller than the distance between two Fe steps, it is likely that the frustration reaches the Mn film surface (Berger and Fullerton, 1997; Berger and Hopster, 1994).

Figure 3b and c show Sp-STM images of the topography and the corresponding spin signal of a 6.9 ML Mn film grown over monatomic steps of the Fe substrate. In the topography, three buried Fe steps are visible indicated by the black arrows. The Mn coverage changes by one ML on both sides of the step edges which is clarified by the numbers presenting the different Mn layers. In the spin signal, the layer-wise antiferromagnetic order between neighboring Mn layers separated by monatomic Mn steps is visible. In addition, magnetic frustrations are visible in the regions above the buried Fe step edges, each separating the Mn film into two domains. Along the three buried Fe step edges, a reversal of the spin contrast appears. In these regions the spin polarization of the Mn rotates by 180°. In the areas indicated by A and B (Fig. 3b,c), the coverage changes from 6 to 7 ML Mn and from 7 to 8 ML along the same buried Fe step edge. As a conse-

<sup>&</sup>lt;sup>1</sup>Around each step on the surface, a contrast is visible in the spin signal (Fig. 2c). In general, such cross talk of the topographic signal in the spin signal was always visible at the position of step edges but the size and the spatial extension change depending on the tip apex.





a)

Fig. 2. (a) Sketch of the magnetic order of Mn on Fe(001). The ferromagnetic Fe substrate and the antiferromagnetic order between adjacent Mn layers is indicated by different gray levels and arrows. Topography (b) and corresponding spin signal (c) of 11.9 ML Mn on Fe (001) measured with the Sp-STM.

Fig. 3. (a) Schema of Mn layers overgrowing an Fe substrate step. Above the buried Fe step edge, a magnetically frustrated region occurs. Sp-STM image of the topography (**b**) and corresponding spin sig-nal (**c**) of 6.9 ML Mn on Fe(001). Three buried Fe step edges are running almost vertically through the images, indicated by black arrows. The layer-wise antiferromagnetic order and the rotation of the magnetization of 180° above the buried Fe step edges is visible (e.g., at point A and B). The different Mn layer thicknesses are indicated by numbers in b.



frustrated region

quence of the layer-wise antiferromagnetic order, the contrast is reversed. Identical situations occur at other areas in this image. The magnetically frustrated regions are similar to  $180^{\circ}$  domain walls in the antiferromagnetic film but they are pinned at the Fe substrate step edges.

The observation of the magnetically frustrated regions at the surface of thin Mn films at the position of buried Fe step edges indicates that the magnetic frustrations are extended throughout the whole Mn film down to the interface, as schematically shown in Figure 3a. This implies that the coupling energy at the interface between Fe and Mn is higher than the domain wall energy in the Mn film, which is likely for thin films. However, Sp-STM is highly surface sensitive so that the behavior within the Mn film is not accessible.

A closer look at the region above a buried Fe step edge allows the study of the magnetic behavior of the magnetic frustration in more detail. A magnified image of such a region is shown in Figure 4a (topography) and b (corresponding spin signal). Here, one buried Fe 1

n=12

frustrated region

40

10

12

14

16 18

50 60 70

12.5 ±1 ML

4.6±0.2 nm



Fe step edge is running almost vertically through the center of the images, indicated by arrows. (c) Sketch of the cross section along the black line in a. (d) Line profile taken along the black line in a showing a monatomic Mn step and a step of subatomic height formed by a buried Fe step. (e) Line profile (averaged over 70 lines) across the magnetically frustrated region in the Mn over-layer at the position of the green box in **b**. The solid line represents a fit of a *tanh*-function to the wall profile. [Color figure can be viewed in the online issue. which is available at www. interscience.wiley.com.] step edge is running almost vertically through the cen-

ter of the imaged area (black arrows as guideline). The line profile in Figure 4d taken along the black line in Figure 4a shows a step of monatomic height between two different Mn terraces ( $\approx 0.16$  nm) and a step of subatomic height ( $\approx 0.018$  nm) at the position of a buried Fe step edge due to the different lattice constants of Fe and Mn. In Figure 4b, clearly the layer-wise antiferromagnetic order between the Mn islands and the Mn layer underneath is visible. Following the way of the buried Fe step edge, a magnetically frustrated region is present in the spin signal. Figure 4e depicts an averaged line profile across the topologically enforced magnetic frustration at the position of the green box in Figure 4b. The measurements indicate that the magnetic frustration has a certain lateral extension.<sup>2</sup> To estimate the wall width at the surface, the experimental profile is fitted with a *tanh*-function. This function is the analytical solution for a one dimensional domain wall neglecting dipolar energies (Hubert and Schäfer 1998). The tanh-function is plotted as a solid line in Fig. 4e and it reproduces the shape of the transition region well. Due to the good agreement, this function is used to determine the wall width which is in this case  $4.6 \pm 0.2$  nm.<sup>3</sup>

The width of the magnetically frustrated regions was studied for several Mn film thicknesses. An Sp-STM image of the thinnest Mn film (2.7 ML) on which a spin contrast was obtained, is presented in Figure 5. In this image, four Mn terraces and two buried Fe steps are visible in the topography (Fig. 5a); the latter are indicated by arrows. In this case, n Mn layers plus 1 ML Fe appear higher in the topography than n + 1 ML Mn, because the out-of-plane lattice constant for thin Mn films, up to 2 or 3 ML, is smaller than that of Fe. This reverses for thicker Mn films, where the out-of-plane lattice constant is larger than that of Fe. This observation is in agreement with the increase of the out-of-plane lattice constant of Mn for thicker films (Kim et al. 1996). Beside the monatomic steps between Mn terraces and subatomic steps, formed by underlying Fe steps, small patches are imaged on the Mn terraces (Fig. 5a). They have a width of about 10 nm and a height of about 50 pm and are more frequently found close to the edges of Mn terraces. From the literature, it is known that Mn intermixes with Fe for substrate temperatures above 370 K during Mn deposition (Bischoff et al., 2002). Thus, most likely these islands are created by interdiffusion. Note on this thin Mn film, the small patches are likely due to intermixing, whereas the small rectangular islands of thicker films are related to the phase transition of Mn.

C)

Since the spin signal contains only changes in the spin polarization, the spin polarization at the sample surface of the intermixed and alloyed layers can be imaged. In the corresponding spin signal (Fig. 5b), the layer-wise antiferromagnetic order and the formation

<sup>&</sup>lt;sup>2</sup>Note that this width is not determined by the lateral resolution of the Sp-STM. The resolution is much better, as will be shown later.

<sup>&</sup>lt;sup>3</sup>The weak, regular pattern visible in the topography and in the spin signal (Fig. 4) is caused by noise. The frequency of this noise level is between 20 and 30 Hz and originates most likely from mechanical vibrations of the STM. The mean amplitude is about 23 pm. In addition, again the contrast at the step edges is visible. Nevertheless, no cross talk is visible in the spin signal at the position of subatomic steps at the position of buried Fe step edges.

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Fig. 5. Sp-STM image of the topography (**a**) and the corresponding spin signal (**b**) of 2.7 ML Mn on Fe(001). The black arrows indicate the positions of buried Fe step edges. (**c**) Line profile taken across a magnetically frustrated region at the position of the green box in **b**. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

of a magnetic frustration along the buried Fe step edges are visible. We analyzed the width of the magnetically frustrated region between the second and third ML Mn. The line profile presented in Figure 5c was taken at the boxed area in Figure 5b where no changes of the contrast due to intermixing were observed. For this a thin Mn film we found a wall width of only 1.2 nm. This is the sharpest magnetic feature we found on Mn films on Fe(001). From the line profile, one can see that the lateral resolution of the Sp-STM is at least 1.2 nm.

A selection of several line profiles obtained across magnetically frustrated regions in Mn films having different thickness (see Fig. 6) clearly shows a widening of these regions with increasing Mn film thickness. The smallest width of 1.2 nm was imaged between the second and third ML Mn and the widest one of 6.9  $\pm$  0.3 nm between 18 and 19 ML Mn. Thicker Mn films could not be investigated due to the phase transition to  $\alpha$ -Mn resulting in a three-dimensional growth and rough surfaces.

The wall width across buried Fe step edges was determined for the six different Mn film thicknesses presented in Figure 6. The widths of the magnetically frustrated regions were always extracted by fitting the experimental line profiles averaged over 25 to 70 lines with a tanh-function. Figure 7 shows the width of magnetically frustrated regions as a function of the Mn film thickness. Since the wall occurs between two different Mn layers, i.e., n and n + 1, we followed the nomenclature of Stoeffler and Gautier (1995) and plotted the value of the wall width at the position of n + 0.5 ML Mn. The error bars in the Mn thickness result from the uncertainty of the evaporation rate. Figure 7 shows that the wall broadens linearly with increasing Mn film thickness, as indicated by a linear function fitted to the experimental data (Schlickum et al., 2004). This behavior of the

widening of magnetically frustrated regions with increasing Mn film thickness is discussed in more detail in the following section.

#### DISCUSSION

Neglecting the dipolar energy, the width of a  $180^{\circ}$ domain wall in a ferromagnet is determined by a competition between the exchange energy and the magnetic anisotropy energy and is given by  $2\sqrt{A/K}$ , where A is the exchange and K the magnetocrystalline anisotropy. The bulk domain wall width for the cubic itinerant ferromagnets is between 20 and 80 nm (Jiles, 1996). For antiferromagnets, a similar relation is expected, as it is well justified to neglect the dipolar energy. For antiferromagnetic bulk Cr, a wall width of about 120 nm (Kleiber et al., 2000) has been found. Assuming an antiferromagnetic exchange proportional to the Néel temperature and a Mn anisotropy similar to that of the 3d ferromagnets, one expects the same order of magnitude for the bulk domain wall width in Mn between 20 and 60 nm. For the following arguments, the exact knowledge of the bulk domain wall width is not needed. The pinned domain walls in thin Mn layers across buried Fe step edges result in a narrow frustration at the surface between the second and third Mn layer of 1.2 nm. The driving force for widening of the magnetic frustration for thicker Mn films is the exchange energy that is gained by approaching the bulk domain wall configuration. Thus, the width of the magnetically frustrated region should asymptotically approach its bulk wall width with increasing film thickness. As expected, we observed a widening, but it is linear with no sign of saturation. This is in agreement with the relatively narrow walls when compared to the expected bulk wall width.

Interestingly, we found a slope of the linear widening, which is close to 2, meaning that the wall width



Fig. 6. Six line profiles across magnetically frustrated regions in Mn films of different film thicknesses. The film thickness is presented by n + 0.5 ML and the wall width in nm; both are indicated in the images.

ż à 6

increases nearly twice as fast as the film thickness. In Figure 7, the experimental wall width is presented together with the linear function having a slope of 2 (red dotted line).

spin signal (%)

ò

ż 4

The slope of the widening of the magnetically frustrated region can be explained within a continuum model in which the exchange is assumed to be isotropic. In a similarly frustrated ferromagnet, this would mean that the pinned wall widens isotropically when increasing the distance from the perturbation. Considering a layer-wise antiferromagnet as a ferromagnet where only the magnetization of every second layer is rotated by 180°, a similar homogeneous widening would be expected for the pinned walls in Mn films at Fe steps. In the case of Mn, this would mean that the ferromagnetic exchange energy within one Mn layer is equal to the antiferromagnetic exchange energy between adjacent Mn layers. The energy needed to turn the magnetization in one point away from its equilibrium state is then only a function of the distance to the neighboring exchange coupled points. This results in a widening of the magnetically frustrated region with an angle of  $45^{\circ}$  and corresponds to a linear widening having a slope of two.

The linear fit to the experimental data has a slope of 2 but a constant offset occurs to the expected linear function. This may have several reasons. First, the frustrated region in the Mn induces a torque on the Fe moments at the interface via the exchange interaction. This may induce a tilt of the Fe magnetic moments near the step edges. Some of the exchange energy caused by the frustration would then be transferred to the Fe and would widen the magnetic frustration in the Mn film. Second, the Sp-STM has a finite resolution that can lead to a widening in the measured Mn wall profile, especially for narrow walls.

The Heisenberg model, which considers the interaction of spins within the exchange coupled system, may



position [nm]

Fig. 7. The width of magnetically frustrated regions of Mn surface layers as a function of the Mn film thickness in ML (bottom scale) and equivalent in nm (top scale). The solid line is a linear fit to the experimental data points. The dotted line is a linear function having the slope of twice the film thickness.

provide a more detailed description of the magnetic frustration. This model in particular is useful due to its simplicity. However, one should keep in mind that localized magnetic moments are considered, which is at most a crude approximation for the itinerant magnetic materials like Fe and Mn due to the delocalized nature of the electrons. As shown in Pajda et al. (2001), one possibility is to use an effective Heisenberg model to describe approximately the magnetic interaction in itinerant materials. The itinerant exchange is considered in an effective exchange coupling constant.

To calculate the width of the magnetically frustrated region in the Mn film on Fe(001), an effective Heisenberg model with classical spins is used and in addition, a fourfold magnetic anisotropy is included. The energy of the system can be written as:

$$E = -\frac{1}{2} \sum_{i,j \neq i} J_{ij} \cos(\theta_{ij}) + \sum_{i} K_i \sin^2 \varphi_i \cos^2 \varphi_i.$$
 (2)

For the calculations, a constant magnetic moment is assumed in each of the two materials (Fe and Mn).  $\theta_{i,j}$ is the relative angle between the directions of the magnetic moments *i* and *j*.  $\varphi_i$  is the angle between the magnetic moment *i* and the direction of the easy axis of the Fe substrate magnetic moments, and  $K_i$  is the anisotropy constant. This means, only a rotation completely in-plane or out-of-plane is allowed and no difference occurs between these two cases because dipolar interactions are neglected. Thus, a Néel wall and a Bloch wall are energetically degenerate. To determine the numerical solution, the angles of the magnetic moments are varied to find the minimum energy configuration.

The values for the exchange coupling constants and the anisotropy constant are well known for bulk bcc Fe. Pajda et al. (2001) calculated J up to the tenth nearest neighbor. The main contributions are given by the nearest and next nearest neighbor, where the next nearest neighbor, has still a contribution of 57% of the nearest one. This is mainly due to the bcc structure of Fe where differences of the distance between the nearest and next nearest neighbor are small (about 13%). The other contributions are less than 13% (Pajda et al., 2001).

For bct Mn, the values for J can only be estimated. The value for the nearest neighbor is determined by assuming a linear dependence between the ordering temperature and the exchange coupling constant (Pajda et al., 2001). The Néel temperature of γ-Mn is  $T_N = 540$  K (Bouarab et al., 1995; Krüger et al., 1996). Using this temperature and J  $\alpha$  T<sub>N</sub>, a value of J = -20 meV is estimated for the nearest neighbor exchange coupling constant. For estimating J for the next nearest neighbor exchange in the Mn film, we assumed a decay of the exchange with increasing distance (r) by . This assumption is based on tight binding calculations (Sutton et al., 1988). We are aware that this is only a rough estimate but ab-initio calculations are not available. The calculated values for the nearest and next nearest neighbor exchange for bcc Fe have decay rates between  $\frac{1}{r^3}$  and  $\frac{1}{r^5}$  (Morán et al., 2003; Pajda et al., 2001) which supports the assumption. Using this approximation and considering the tetragonal distortion in the Mn film, we obtained a next nearest neighbor coupling constant of J = 12 meV for the in-plane exchange and J = 7 meV for the out-of-plane exchange. The coupling of next nearest neighbors is assumed to be ferromagnetic. At the interface between Fe and Mn, the same exchange values are assumed as used in the Mn film.

The choice of the exchange coupling constants is summarized graphically in Figure 8, where the three dimensional structure is projected into a two-dimensional plane, for simplicity. The first Mn layer is



Fig. 8. (a) Lattice structure of bct Mn on Fe projected in the (100) plane. The exchange coupling constants used in the calculations are indicated by numbers. (b) Starting configuration for the calculations in a Heisenberg model. The different gray levels of the localized magnetic moments are correlated to the Fe substrate and the layer-wise coupling of the Mn layers. The arrows represent the direction of the magnetic moments parellel or antiparallel to the Fe one and the dots and crosses the ones having an angle of  $\pm 90^{\circ}$ .

assumed to couple ferromagnetically to the Fe layer. For the anisotropy, the value for bulk Fe is given by  $K_i = 4 \mu eV$  (Escudier, 1975.) In the case of thin Mn films, we are in the limit where the magnetically frustrated region is much thinner than a bulk domain wall. While in the latter case, the width is determined by the equilibrium between the exchange and the anisotropy energy, in thin films the width is dominated by the exchange interaction being much higher than the anisotropy energy. Therefore, the anisotropy can be neglected in the Mn film. To confirm this approximation, test calculations were performed choosing different realistic values for the anisotropy in the Mn flim. No changes occurred in the width of the calculated magnetically frustrated region. However, the anisotropy cannot be neglected in the Fe substrate due to the fact that the anisotropy limits the propagation of the magnetically frustrated region into the Fe substrate.

The starting configuration for the minimization of the energy is presented in Figure 8b. The Fe film is homogeneously magetized and consists of 70.5 ML. No influence of the magnetically frustrated region was found for thicker Fe films. The thickness of the Mn film is varied between 2.5 and 20.5 ML and an atomically sharp 180° wall is placed above an Fe step edge having the same width in every Mn layer. To check the influence of this starting configuration, several different starting arrangements were chosen. For one configuration, no magnetic frustration was inserted in the Mn film. The result and especially the calculated width of the magnetically frustrated region were found to be independent of the starting configuration, though the calculation time was significantly increased in some cases. Therefore, the above-mentioned starting configuration, which is already close to the energy minimum, was chosen.

Figure 9 shows the result of the calculation of a magnetically frustrated region of 20.5 ML Mn. The result is presented in a two-dimensional plot together with the underlying Fe substrate. In the calculations, the nearest neighbor and next nearest neighbor exchange interaction was considered. Black and white areas corr- espond to MLs where the magnetic moments have an angle of  $180^{\circ}$  and  $0^{\circ}$  compared to



Fig. 9. (a) The calculated angle distribution  $(\phi)$  of the local magnetic moments projected along the direction of the undisturbed Fe moments above and below an Fe step edge of a 20.5-ML-thick Mn film. The first layers showing the alternating contrast present the antiferromagnetic order of adjacent Mn layers. The Fe magnetic moments below the step edge of a is shown in **b** with a considerably increased contrast (about 95%).

the direction of non-tilted Fe magnetic moments. The rotation of the magnetic moments in the magnetically frustrated region is visible and the calculations show that the frustration is localized above the Fe step edge (Fig. 9a). Figure 9b displays only the Fe film with enhanced contrast (more than 95%) to show the weak tilt of the Fe magnetic moments. The induced rotation of the Fe moments is at most 36° in the topmost Fe layer close to the step edge, and it is already reduced to about 7° in a distance of 30 atoms in the plane away from the Fe step edge. In the 10th layer below the step, the rotation is reduced to  $12^{\circ}$ . The size of the rotation of the Fe moments depends strongly on the Mn coverage. For low coverage, nearly no rotation is found. From this model, we see that the magnetic frustration in the Mn film induces a torque on the Fe moments due to the exchange that results in a tilt of the Fe moments near the Fe step edge. This means that a topological defect can be associated with a long-range effect extending into the whole antiferromagnetic Mn film and into the ferromagnetic substrate. Calculations performed by Stoeffler and coworkers showed a similar behavior for Cr films overgrowing an Fe step edge (Robles et al., 2003). In the calculations, it was found that the magnetic defect line extends into the whole Cr film and that the magnetic moments of the underlying Fe substrate are tilted close to the Fe step edge.

In Figure 10a, a calculated line profile taken at the topmost Mn layer in Figure 9a, is shown. To determine the calculated wall width of the magnetically frustrated region, the curve was fitted with a *tanh*-function as in the case of the measured data. A good agreement between the calculated wall profile and the behavior of a *tanh*-function was found (red dots).

Figure 10b shows the width of the magnetically frustrated region within a 20.5-ML-thick Mn film from the interface to the Mn surface layer (dashed line). The wall width was determined from line profiles within the film presented in Figure 9. A strong widening is found in the first few Mn layers above the interface and only small changes are found close to the surface layer. In this case, the ratio between the exchange coupling at the interface and in the Mn film is  $J_{MnFe}$ /  $J_{Mn} = 1$ . The product of both, the ratio of  $J_{MnFe}/J_{Mn}$ and the film thickness is much bigger than one. For this case, numerical simulations performed by Levchenko et al. (1998) for a general system consisting of a thin antiferromagnetic film on top of a ferromagnetic substrate show a similar behavior of widening of a magnetic frustration within an antiferromagnetic film. In their calculations, a nearest neighbor Heisenberg model was used as a basic model for the simulations. When decreasing the ratio of  $J_{MnFe}/J_{Mn}$ , the numerical simulations of Levchenko and cowokers predict that the shape of the curve stays the same and that the curve is only shifted to higher wall width. By decreasing  $J_{MnFe}/J_{Mn}$  by a factor of four, our calcula-tions yield the curve presented by dots in Figure 10b.



Fig. 10. (a) Calculated line profile projected along the direction of undisturbed Fe moments, taken at the surface of a 20.5-ML-thick Mn film (black line) together with a fit of a *tanh*-function (red dots). (b) The calculated behavior of a wall within a 20.5-ML-thick Mn film for the case that  $J_{Mn}$  is equal  $J_{MnFe}$  (dashed line) and  $J_{MnFe}$  is four times smaller than  $J_{Mn}$  (dotted line).

In agreement with the simulations, the two curves show nearly the same behavior and the one having a low ratio of  $J_{MnFe}/J_{Mn}$  is only shifted to a higher wall width.

In Figure 11, the measured wall widths and the calculated widths are shown. Blue triangles present the case where the energetic minimum of the magnetic frustrated Mn film was calculated by taking into account only the nearest neighbor exchange interaction. The calculated wall widths as a function of the Mn film thickness have a lower slope than the experimentally determined one and the widths of the walls are smaller. In a next step, the wall width was calculated by considering the nearest and next nearest neighbor exchange interaction. The values of our calculations are indicated by red diamonds in Figure 11. The slope is much closer to the linear fit to the experimental data, but still a small offset occurs. The calculated width is again smaller than the experimental one. For both calculations, a ratio of  $J_{MnFe'}J_{Mn} = 1$  was used. The width of the wall obtained for the ration of  $J_{MnFe'}$  $J_{Mn} = \frac{1}{4}$  is presented in orange stars in Figure 11. The agreement to the experimental data is better than in the case that  $J_{MnFe}/J_{Mn} = 1$  (red diamonds), which



Fig. 11. The measured data (green data points) with a linear fit (green line) shown in Figure 7 are presented together with the calculated wall widths of magnetically frustrated regions using the Heisenberg model. The calculated data shown in blue triangles are obtained by considering only the nearest neighbor exchange interaction and in red diamonds by considering the nearest as well as the next nearest neighbor exchange interaction and the bct structure of Mn. Using the same parameter as in the latter case and reducing the exchange at the interface to 25%, one obtains the values presented in orange stars. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

suggests that the exchange interaction at the interface between Fe and Mn may be reduced. This prediction is supported by the observation that at some areas, no magnetic frustrations were found at the surface of a Mn film above a buried Fe step indicating a relatively small interface coupling compared to the exchange of Mn. Taking into account the crude approximations in particular for the exchange in the Mn film and at the interface, the agreement between the calculated wall width and the experimental one is rather satisfying.

The remaining difference between the calculated and experimental widths of the magnetically frustrated region may have several origins. The values for the exchange in the Mn film and at the interface are only estimated values. In particular, the exchange interaction at the interface is a critical parameter.

Since in the experiment the Mn films were deposited on Fe having a temperature of 370 K, intermixing at the interface occurred, which is also not included in the theoretical model. The lattice mismatch (caused by the difference in the out-of-plane lattice constant) at the position where Mn overgrows an Fe step edge is not considered as well. Possible changes of the exchange interaction or of magnetic moments close to the surface and interface are neglected. Several of the above-discussed considerations can be taken into account by ab-initio calculations. Therefore, these calculations would be highly desirable for this system. Both models, the Heisenberg model and the continuum model, describe the widening at the surface as rather satisfying. The main difference between these two considerations is the behavior within the Mn film. In the Heisenberg model, a parabolic behavior was found while from the continuum model a linear widening is expected within the Mn film. The behavior within a Mn film is not accessible with Sp-STM measurements.

### CONCLUSIONS

The capability of the Sp-STM was used to measure the spin arrangement of antiferromagnetic surfaces with a high lateral resolution of at least 1 nm. The layer-wise antiferromagnetic ordered Mn films, which are in direct contact with a ferromagnetic Fe(001) substrate, were investigated. It was confirmed that Mn shows a layer-wise antiferromagnetic order between adjacent layers. Magnetically frustrated regions were found at the surface of Mn films on Fe(001). The magnetic frustrations are explained by the interface roughness between Mn and Fe. When Mn is overgrowing a monatomic Fe substrate step, the Mn layer thickness is different by one atomic layer on both sides of the step. Assuming the same magnetic coupling between Mn and Fe on both sides of the step edge, the layer-wise antiferromagnetic order within the Mn film cannot be fulfilled on both sides of the step without creating a magnetic frustration. The investigation of the spin arrangement influenced by monatomic steps has been beyond the resolution limit of the established magnetic imaging techniques. Here, Sp-STM provides an ideal tool to probe the behavior of single, laterally confined magnetic frustrations. The possibility to image the topography and the magnetic signal simultaneously allows the correlation between magnetic structures and specific topographic features. By investigating the width of the magnetic frustrations as a function of the Mn film thickness, a linear widening with increasing Mn thickness was observed. A width of the magnetically frustrated region between 1 nm (between the second and third ML Mn) and 7 nm (between the 18 and 19 ML Mn) was found. The experimental widening of the magnetic frustration with increasing Mn film thickness was compared to two model descriptions, a continuum model and calculations based on a Heisenberg model. Both models reproduced the observed widening of the magnetic frustrations at the Mn surface with increasing film thickness rather satisfying. However, the behavior within the Mn films is significantly different for both models. Since Sp-STM is only sensitive to the surface layers, only the behavior at the Mn film surface could be investigated.

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