# Step-Induced Frustration of Antiferromagnetic Order in Mn on Fe(001)

U. Schlickum, N. Janke-Gilman, W. Wulfhekel, and J. Kirschner
*Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany*
(Received 21 May 2003; published 12 March 2004)

We studied the spin arrangement in ultrathin antiferromagnetic Mn films in contact with a ferromagnetic Fe(001) substrate using spin-polarized scanning tunneling microscopy. Mn shows a layerwise antiferromagnetic order on Fe(001). In regions where Mn overgrows Fe steps, a frustration of the antiferromagnetic order occurs which is similar to a 180° domain wall. This topologically enforced frustration was studied as a function of Mn thickness. A linear increase of the width of the frustration region with the Mn thickness was found.

DOI: 10.1103/PhysRevLett.92.107203 PACS numbers: 75.70.–i, 68.37.Ef, 75.50.Ee, 75.60.Ch

When an antiferromagnetic film is grown on a ferromagnetic surface, complex frustrations of the antiferromagnetic order are induced in the film. These frustrations are caused by the exchange interaction at the interface and the unavoidable atomic roughness of the ferromagnet disturbing the antiferromagnetic order at step edges [1–4]. The detailed structure of these frustrations has been out of reach of the established magnetic imaging techniques due to their limited lateral resolution. Most of our knowledge on bulk antiferromagnets has been gained by scattering methods, i.e., neutron scattering [5], that are sensitive to periodic structures. Because of the localized nature of frustrations, scattering methods have not been successful to clarify the spin configuration in these frustrations. With the development of spin sensitive scanning tunneling microscopy [6,7] new imaging tools are now available to resolve the fundamentally interesting structure of frustrations and open a new field of research. Besides the fundamental interest, frustrations play an important role in applications. While the exchange coupling across the ferromagnet/antiferromagnet interfaces, e.g., in Fe/Cr/Fe sandwiches, has been frequently used [8], the detailed spin structure at the interfaces and surfaces on the local scale are still unknown. Knowledge of the spin arrangement would reveal the physical mechanisms operating.

As a simple model system for topologically induced frustrations, we chose the layered antiferromagnet Mn(001) grown on Fe(001). This material system is prototypic for most layered and uncompensated antiferromagnets, e.g., Cr(001) [9] or NiO(111) [10]. Mn in contact with Fe(001) has been studied by a variety of different methods. By spin-polarized electron energy loss spectroscopy, a layer-by-layer antiferromagnetic coupling of Mn on Fe(001) was found [11]. This behavior of a topological antiferromagnet was also observed with scanning electron microscopy with polarization analysis [12]. The coupling within a Mn atomic plane is ferromagnetic, while normal to the surface a layerwise antiferromagnetic ordering with in-plane spin polarization was observed. Recently this antiferromagnetic behavior was also measured with spin-polarized scanning tunneling spectroscopy (Sp-STS) [13] and spin-polarized scanning tunneling microscopy (Sp-STM) [14]. Figure 1 shows a schematic model of the topographic and magnetic behavior of Mn layers on Fe(001). The antiferromagnetic coupling between adjacent Mn layers is indicated by arrows pointing in opposite directions. Where Mn overgrows a step edge of the underlying Fe substrate, the thickness of the Mn layer on one side of the step edge is one atomic monolayer (ML) higher than on the other side (see Fig. 1). Assuming either ferromagnetic [15] or antiferromagnetic [16] coupling at the interface between Mn and Fe, the in-plane Mn ferromagnetic coupling in combination with interplanar antiferromagnetic ordering leads to a conflict at the Fe step edge. This results in a frustrated zone in the Mn film. Theoretically these frustrations were first proposed for the similar system Cr/Fe(001) [1–4] and were described as 180° domain walls in the antiferromagnet. In Fig. 1 the frustrated region in the Mn layers across a buried Fe step is indicated as a transition region. In this Letter we study this frustration in real space with high resolution Sp-STM as a function of the thickness of the antiferromagnetic film and reveal the evolution of the frustration from a line defect at the step towards an extended frustration.

Mn grows in a Stranski-Krastanov mode on Fe(001), i.e., after a flat wetting layer, three-dimensional growth sets in. The wetting layer is present in the pseudomorphic body centered tetragonal structure [17], i.e., the in-plane lattice constant of Mn is equal to that of Fe ($a = b =$ 0.287 nm) and the out-of-plane lattice constant is expanded ($c = 0.323$ nm) compared to Fe ($c = 0.287$ nm)


FIG. 1. Schematic model of a frustration zone in the antiferromagnetic Mn across an underlaying Fe step edge.

  

[18–21]. Depending on the growth conditions, dislocation formation, three-dimensional growth, and phase transition set in between 3 and 25 ML [18,21,22]. These appear as small islands in STM scans [17]. Because of the difference of the out-of-plane lattice constant between Fe and Mn, the buried substrate steps are visible in the topography as weak steps of subatomic height ($n + 1$ ML Mn are higher by 0.018 nm compared to $n$ ML Mn plus 1 ML Fe) [17], as indicated in Fig. 1.

Mn films were deposited in ultrahigh vacuum ($p < 1 \times 10^{-10}$ mbar) on clean, high quality Fe(001) surfaces of Fe whiskers by electron beam evaporation with growth rates of $\approx 0.5$ ML/min at 370 K. The film thickness was monitored by medium energy electron diffraction (MEED) during film growth and was cross-checked with topographic STM measurements to determine the Mn coverage. Sp-STM measurements were carried out on domains of the Fe whisker much larger than the scanning area. *In situ* magneto-optical Kerr microscopy of the Fe whisker was used to confirm the magnetic ground state consisting of a 180° domain wall along the long axis of the Fe-whisker and end domains [14]. In this configuration, the magnetization at the Fe-whisker surface lies in plane and along the long axis. Topographic and spin resolved STM images were obtained *in situ* at 300 K at a bias voltage of 0.1 V and a feedback current of 3 nA.

In the experimental setup, in-plane spin sensitivity was obtained with an Sp-STM electrode consisting of a soft magnetic ring of CoFeSiB with a small coil around it. The magnetization of the ring is periodically switched with an ac current while the tunneling current is measured [14]. The tunneling current depends on the relative orientation of the ring and the sample spin causing modulations of the tunneling current due to the tunneling magnetoresistance effect [23]. The average tunneling current ($\bar{I}$) for both ring magnetizations is used to obtain the topographic image. $\bar{I}$ contains no information on the spin. The difference in tunneling current ($\Delta I$) for opposite ring magnetization is detected with a phase sensitive lock-in amplifier. $\Delta I$ depends only on the spin and contains no topographic information. The difference is proportional to the spin polarization of the sample projected along the ring tangent. With this configuration, one well-defined in-plane component of the sample spin polarization can be imaged at the same time as the topography. In all measurements the magnetization of the ring was collinear to the magnetization of the Fe whisker. In contrast to Sp-STS, where spectroscopic details of the differential conductance—containing both spin dependent and independent information—are used to obtain magnetic sensitivity [6], Sp-STM separates the spin dependent contributions of the tunneling current from those that are spin independent [14].

Figure 2(a) shows the topography of 6.9 ML Mn on Fe(001). One can see terraces and islands with step edges of monatomic height. This is indicative of a mixed step flow and island nucleation growth mode. Because of the step flow, evaporated Mn overgrows buried Fe steps. Therefore, $n$ layers Mn were grown on the upper side of the Fe substrate steps and $n + 1$ layers on the lower side. Three of these buried Fe steps are visible in Fig. 2(a), indicated by the arrows. According to the model in Fig. 1, successive Mn layers should be oppositely magnetized. This layerwise antiferromagnetic coupling can be observed in Fig. 2(b), where adjacent Mn layers couple antiferromagnetically (black and white areas). This is in

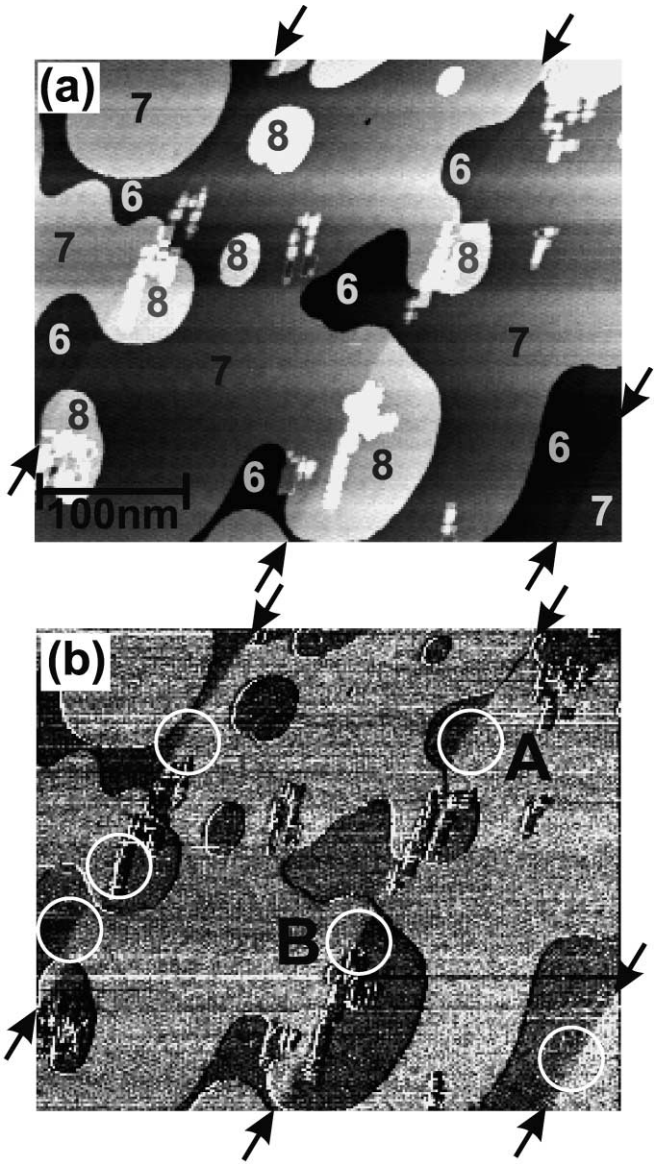


FIG. 2. Sp-STM image of (a) the topography and (b) the corresponding spin signal of 6.9 ML Mn on Fe(001). In the spin signal, the alternating contrast represents the antiferromagnetic coupling between adjacent Mn layers. The three lines running vertically through the images signify step edges in the underlying Fe substrate, indicated by arrows. The different Mn layers are indicated by numbers in (a).

agreement with observations of Yamada *et al.* [13]. Additionally, a domain wall along the three buried Fe step edges is visible. In the region, indicated by white circles *A* and *B*, the coverage changes from 6 to 7 ML Mn and from 7 to 8 ML along the same Fe step edge. As a consequence of the layerwise antiferromagnetic coupling the contrast across the domain wall reverses. Similar cases are marked by further white circles. The formation of the frustrations in the Mn film results from the fact that the coupling energy at the interface of Fe and Mn is higher than the domain wall energy in the Mn film. This behavior was found for all Mn thicknesses investigated in this work.

Figure 3 shows a zoom into a frustrated region in the Mn layer across an Fe step edge. In this case, 11.9 ML Mn were deposited on Fe(001). The Fe step edge is running almost vertically through the center of the images [Figs. 3(a) and 3(b)], as indicated by the arrows. It appears in the line scan as a small step of $0.027 \pm 0.01$ nm [Fig. 3(c)] at the position of 0 nm [24]. The step height is the difference between the out-of-plane lattice constant of Fe and Mn. In the corresponding spin signal [Fig. 3(b)] the antiferromagnetic coupling between the Mn islands and the underlaying Mn layer can be seen [25]. Following the way along the buried Fe step edge a reversion of contrast in the Mn spin signal can be seen. This contrast is opposite on the islands and the closed layer underneath, as discussed above. A line profile across this topologically enforced 180° domain wall is shown in Fig. 3(d). The contrast in the spin signal $\Delta I/\bar{I}$ across the domain wall is about 0.9%. For the other measured thicknesses similar contrasts were found. The width of the frustrations at the surface is estimated by fitting the standard wall profile for uniaxial systems [26] to the experimental line profiles:

$$m(x) = \tanh\left(\frac{x}{w}\right), \tag{1}$$

where the domain wall width is given by $2w$. This function reproduced well the shape of the transition region [see Fig. 3(d)]. For the line profile of this figure, the extracted domain wall width is $4.55 \pm 0.54$ nm. Thus, the spin polarization does not change abruptly, but a domain wall of several nm width is formed. The width is much larger than the lateral resolution of the Sp-STM of 1 nm or better [14].

The domain wall width across buried Fe step edges was determined for six different Mn thicknesses. Always a line profile averaged over 25 to 70 lines was fitted with Eq. (1). The values of the domain wall width as a function of Mn thickness are shown in Fig. 4 [27]. The domain wall occurs between two different Mn layers $n$ and $n + 1$. Following the nomenclature of Stoeffler *et al.* [3] the value of the domain wall width was plotted at the position of $n + 0.5$ ML Mn, where $n$ is an integer. The error bars in the Mn thickness result from the uncertainty of the evaporation rate as determined by MEED. Clearly, a widening of the frustrated region with increasing Mn thickness is visible. A widening as a function of film thickness was theoretically proposed for Cr on Fe(001) [3]. Because of the similar magnetic behavior of Cr and Mn, a widening of the enforced Mn domain wall is also expected. The solid line represents a linear fit to the

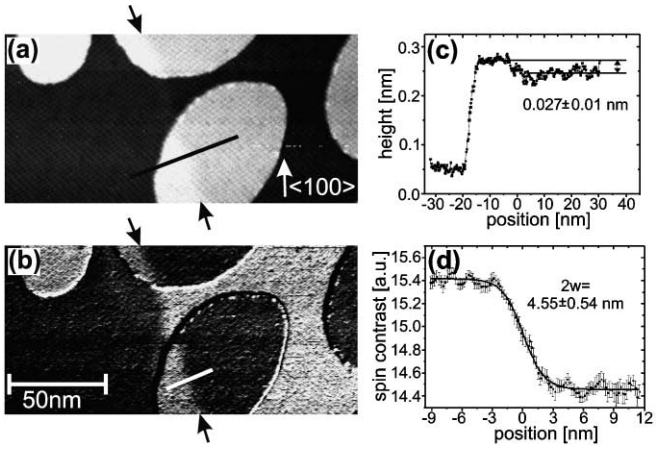


FIG. 3. Sp-STM image of (a) the topography and (b) the corresponding spin signal of 11.9 ML Mn on Fe(001). The line running vertically through the center of the topography image signifies a step edge in the Fe substrate, and appears as a small step in the Mn overlayer (c). (d) Line profile (averaged over 70 lines) across the frustrated region in the Mn overlayer between 12 and 13 ML. The error bars represent the standard deviation. The solid line represents a fit to the wall profile. Line scans (c) and (d) are taken along the lines indicated in (a) and (b).

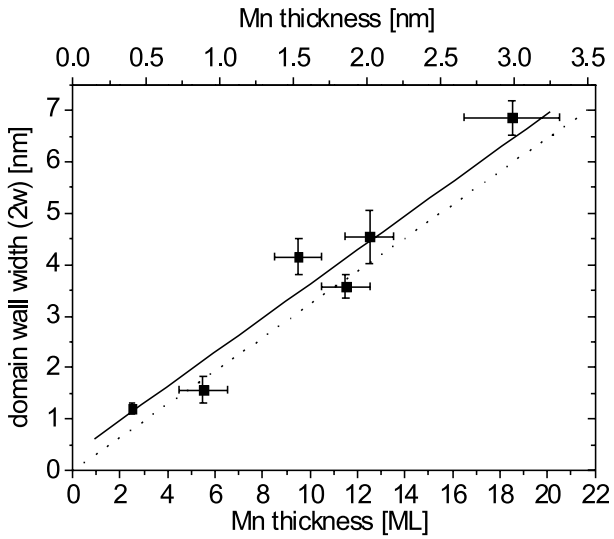


FIG. 4. The data points represents the domain wall width of the topological enforced domain wall in the Mn overlayers as functions of the film thickness in ML and equivalent nm. The solid line is a linear fit to the experimental data. The dotted line is a linear function with the slope of twice the film thickness.

measured data points. The linear dependence describes the experimental data well.

In bulk antiferromagnets, the width of a 180° domain wall is determined by a competition between the exchange energy and the magnetic anisotropy ($K$) and is given by $2\sqrt{A/K}$ [26], where $A$ is the exchange constant within the antiferromagnet. For the cubic itinerant ferromagnets the bulk wall width is estimated between 30 and 200 nm [28] and for Cr about 120 nm [29]. The domain wall in thin Mn layers across an Fe step edge is a consequence of pinning of the Mn spin by the Fe substrate. This results in a narrow frustration at the surface of 1.2 nm width between the second and the third ML Mn. When increasing the Mn thickness, the widening of the frustration at the surface results from balancing the energy gain of approaching the bulk domain wall width and the cost due to the exchange interaction to the underlaying Mn layers. The width of the frustration should approach the bulk wall width in an asymptotic manner. In our experimental data, however, we see a linear increase but no saturation. This can be explained by the fact that the wall width is far away from the bulk value. Experimentally it is not possible to determine the domain wall width for films thicker than 20 ML because of the phase transition to $\alpha$-Mn. Interestingly, the slope of the linear increase is close to 2, i.e., the wall width $2w$ is nearly equal to twice the film thickness. This slope can be explained on the basis of a simple continuum model. In this model there is an exchange energy between the magnetization of two points in the Mn film. The energy needed to turn the direction of magnetization in one point away from its antiferromagnetic ground state is just a function of the distance between the two exchange coupled points. In such an isotropic system, the line defect at the step edge is isotropically smoothed out in the Mn layer. As a consequence of this, a slope of 2 is predicted. This behavior is indicated as a dotted line in Fig. 4. The fitted line to the experimental data, however, lies slightly above the simple continuum model. This might be due to two effects. First, the frustrated region in Mn induces a torque on the Fe moments at the interface due to the exchange, possibly inducing a tilt of the Fe moments near the step. By this, some of the energy of the frustrated system is transferred to the Fe exchange and the Mn wall widens slightly. Second, the Sp-STM has a finite resolution which can lead to a widening in the measured Mn wall profiles, especially for narrow walls [30].

In conclusion we showed that Sp-STM allows a view into the coupling behavior at the interface between a layered antiferromagnet and a ferromagnet on the nanometer scale. The investigation of the spin arrangement showed a frustration in the antiferromagnetic Mn(001) films along buried step edges of the Fe(001) substrate. The frustration resembles a 180° domain wall which broadens linearly at the surface with increasing Mn film thickness. The results obtained for the model system Mn/Fe(001) should qualitatively hold for other layered antiferromagnets like Cr(001) or NiO(111). We analyzed the structure of the frustrations at step edges which are of importance in exchange coupling, e.g., in Fe/Mn/Fe or Fe/Cr/Fe structures.

[1] A. Berger and H. Hopster, Phys. Rev. Lett. **73**, 193 (1994).
[2] A. Vega *et al.*, Phys. Rev. B **51**, 11 546 (1995).
[3] D. Stoeffler and F. Gautier, J. Magn. Magn. Mater. **147**, 260 (1995).
[4] A. Berger and E. Fullerton, J. Magn. Magn. Mater. **165**, 471 (1997).
[5] C. G. Shull and J. Samuel Smart, Phys. Rev. **76**, 1256 (1949).
[6] M. Bode, M. Getzlaff, and R. Wiesendanger, Phys. Rev. Lett. **81**, 4256 (1998).
[7] W. Wulfhekel and J. Kirschner, Appl. Phys. Lett. **75**, 1944 (1999).
[8] D. Olligs *et al.*, Europhys. Lett. **59**, 458 (2002).
[9] J. Unguris, R. J. Celotta, and D. T. Pierce, Phys. Rev. Lett. **69**, 1125 (1992).
[10] J. X. Shen and M. T. Kief, J. Appl. Phys. **79**, 5008 (1996).
[11] T. G. Walker and H. Hopster, Phys. Rev. B **48**, 3563 (1993).
[12] D. A. Tulchinsky, J. Unguris, and R. J. Celotta, J. Magn. Magn. Mater. **212**, 91 (2000).
[13] T. K. Yamada *et al.*, Phys. Rev. Lett. **90**, 056803 (2003).
[14] U. Schlickum, W. Wulfhekel, and J. Kirschner, Appl. Phys. Lett. **83**, 2016 (2003).
[15] S. Andrieu *et al.*, Phys. Rev. B **58**, 8210 (1998).
[16] J. Dresselhaus *et al.*, Phys. Rev. B **56**, 5461 (1997).
[17] T. K. Yamada *et al.*, Surf. Sci. **516**, 179 (2002).
[18] S. T. Purcell *et al.*, Phys. Rev. B **45**, 13 064 (1992).
[19] B. Heinrich *et al.*, J. Vac. Sci. Technol. A **5**, 1935 (1987).
[20] S. K. Kim *et al.*, Phys. Rev. B **54**, 5081 (1996).
[21] S. Andrieu *et al.*, Phys. Rev. B **57**, 1985 (1998).
[22] R. Pfandzelter, T. Igel, and H. Winter, Surf. Sci. **389**, 317 (1997).
[23] M. Jullière, Phys. Lett. **54A**, 225 (1975).
[24] The piezo was calibrated on monatomic Fe steps.
[25] A weak contrast appears in the spin signal at the position of monatomic steps in the Mn layer. This cross talk from topography may be caused by the finite response speed of the feedback loop or due to nonperpendicular tunneling between the ring and the sample at the step edge. A similar cross talk is, however, not observed on the buried Fe steps of subatomic height.
[26] A. Hubert and R. Schäfer, *Magnetic Domains* (Springer-Verlag, Berlin, 1998).
[27] We found no dependence of the wall width on the position of the wall on the whisker.
[28] E. Kneller, *Ferromagnetismus* (Springer-Verlag, Berlin, 1992).
[29] M. Kleiber *et al.*, Phys. Rev. Lett. **85**, 4606 (2000).
[30] The real wall width is slightly broadened by the instrument resolution of 1 nm or better.