Magnetic properties of the (100) surface of Fe

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(Received 21 March 1988; revised manuscript received 23 June 1988)

Hysteresis loops taken at a surface are often found to change even when the probing depth of the magnetic measurement varies by only a few lattice spacings. We report an interpretation of these changes in the framework of a simple model which assumes that only one sheet of thickness d at the surface is magnetically different from the bulk. The model reproduces the experimental hysteresis loops with a variety of materials. One obtains the magnetic anisotropy K_s of the surface and the exchange stiffness $A_{1,2}$ along a path perpendicular to the surface. For Fe(100), K_s and $A_{1,2}$ are found to be very small; furthermore, the average easy direction of the surface magnetization is at approximately 75° to the one in the bulk.

Surface magnetism has experienced a rapid development since it became possible to prepare and characterize single magnetic layers; surprising and unexpected results have been obtained. The experiments on (100) surfaces of metastable fcc Fe grown on Cu(100) (Ref. 1) and of stable bcc Fe grown on Ag(100) (Refs. 2 and 3) are particularly important. In contrast to theoretical predictions employing local-density-functional theory,[4] fcc Fe turned out to be ferromagnetic with a Curie temperature of 400 K.[1] Furthermore, at temperatures below 100 K, both types of Fe exhibit magnetic anisotropies that are about 100 times larger than the bulk anisotropy. The possibility of extremely large anisotropies introduced by the reduced symmetry at the surface had been predicted theoretically,[5] yet its absence for one layer but appearance with several layers was surprising.

In view of this situation, it seems appropriate to more closely examine the (100) surface of common bcc Fe for surface-induced anisotropies, as well as anomalous exchange interactions. If phenomena similar to the ones observed with Fe(100) grown on Cu and Ag also occur with Fe(100) on its own proper substrate, the interpretation of surface magnetic measurements will greatly change from what it has been so far.[6] It has, in fact, been shown that anomalies in surface anisotropies and surface-to-bulk exchange interactions may induce special magnetic structures at the surface that are expected to strongly depend on temperature.[7] Therefore, interpretation of surface-sensitive experiments like spin-polarized photoemission[8] may be affected by a change in magnetization direction and altered thermal excitations instead of relating directly to the temperature dependence of bulk magnetism.

At present, the most direct information comes from surface-hysteresis loops. With bulk constants like the exchange stiffness A which is the exchange energy $J\mathbf{S}_1\cdot\mathbf{S}_2$ between two neighboring atoms with spin $\mathbf{S}$ divided by the distance of the atoms, and with the magnetic anisotropy K, the direction of the magnetization should change only over distances of the order of $\sqrt{A/K}$, the width of a domain wall. This is 10–100 nm in most magnetic materials including Fe. Hence, if surface-hysteresis loops are taken with techniques that differ in probing depth by a few lattice parameters only, we expect on the basis of bulk constants that the loops must be identical. However, Allenspach and co-workers[9] observed that the shape of the hystersis loops taken on Fe(100) by measuring the spin polarization of secondary electrons depends on the energy E_S of the secondaries. There are quite convincing general arguments proving that electron-electron scattering in a solid cannot change if a magnetic field of the order of 10 Oe is applied. The altered shape of the loops must come about because the probing depth depends on E_S; the changes of the probing depth, however, are small, of the order of one or two lattice spacings only. If hysteresis loops can change over such small distances, exchange and anisotropy must indeed be very different at the surface compared to the bulk. It is the purpose of this paper to develop a simple model with which one can interpret surface induced changes in hysteresis loops and apply it specifically to the (100) surface of common Fe. We will show that one can, in fact, determine the direction and magnitude of the surface anisotropy, K_S, and obtain estimates for the surface-to-bulk exchange stiffness $A_{1,2}$. The present analysis has already been tested successfully on model interfaces between polycrystalline Fe films of 1–6 nm thickness and amorphous FeTb (Ref. 10) where, however, very different length scales and magnitudes of the magnetic properties prevail.

I. DEVELOPMENT OF THE MODEL

For a first insight into the processes of magnetization reversal near a surface it is advantageous to develop a simple model with few parameters. The experimental results actually suggest the simplest possible model for the case of the Fe(100) surface in which only one sheet of thickness d at the surface is magnetically different from the bulk. If the external magnetic field, H, is applied in the easy direction of magnetization, the anisotropy keeps the specimen in a single-domain state even when H is removed. If H is reversed and reaches the value of the coercive field H_C, a reversed magnetic domain nucleates or grows from a preexisting nucleus prior to coherent ro-

tation of the magnetization M in most cases. The reversed domain expands by domain-wall movement which results in a sudden reversal of M at $H=-H_C$. Therefore, bulk magnetization loops for H along the easy direction are square loops as shown in Fig. 1. If the easy direction varies somewhat throughout the material, wings are observed for $H \leq -H_C$ showing that M tends to finally rotate everywhere into the direction of H. Pierce, Celotta, and Unguris[11] first observed, for the case of the magnetic glass FeBSi, that surface hysteresis loops are different from bulk loops in that they exhibit a rounded edge as $H \rightarrow -H_C$, but no wings once the magnetization has switched as illustrated in Fig. 1. Pierce and coworkers achieved outmost surface sensitivity by measuring the spin dependence of the elastic scattering of spin-polarized electrons from a GaAs source. In elastic scattering, the probing depth is half the electron mean-free path as the electron has to travel in and out of the sample. Furthermore, the mean-free path has a minimum of $\simeq 0.5$ nm for the electron energy of 100 eV used in the above experiment. Hence, one estimates that the probing depth was $\simeq 0.25$ nm, which is about one lattice parameter. Allenspach *et al.*[9] observed the same phenomenon for the (100) surface of Fe, but with a different technique, namely the measurement of the spin polarization of secondary electrons excited with an unpolarized primary-electron beam at an energy of 100 eV. The primary beam penetrates, on the average, $\simeq 0.5$ nm until the first inelastic electron-electron collision takes place. The secondary electrons may undergo elastic scattering with a larger mean free path before escaping. If the energy of the secondary electrons is lowest, namely 1 eV, the probing depth is largest. Abraham and Hopster[12] estimate that the magnetic probing depth of the low-energy-cascade electrons is 3–4 atomic layers with $3d$-transition metals. This estimate is corroborated by spin-polarized photoemission on bcc Fe layers on an Ag substrate[2] since the full saturation polarization is reached already after five monolayers of Fe. If in the experiment of Allenspach *et al.* E_S is increased to 50 eV, the probing depth will be reduced to its minimum value of about one atomic distance similar to the elastic scattering case in the work of Pierce *et al.* Indeed, while at $E_S=1$ eV one still observes the bulk loop, typical surface loops as defined in Fig. 1 appear for $E_S=50$ eV. This suggests that the surface loop is caused by the last or the two last layers only, whereas all deeper layers display bulk loops. The simplest model then assumes a sheet of thickness d of the order of the lattice parameter at the surface which possesses a special magnetization M_S and a uniaxial surface anisotropy K_S. This surface sheet is coupled to the second layer by an exchange interaction $J^*\mathbf{S}_1\cdot\mathbf{S}_2=\xi A_{1,2}$ where $\mathbf{S}_1$ and $\mathbf{S}_2$ are neighboring magnetic moments in the sheet and the first layer of the bulk, respectively, ξ is the distance between the surface sheet and the bulk, and $A_{1,2}$ is the exchange stiffness along a path perpendicular to the surface.

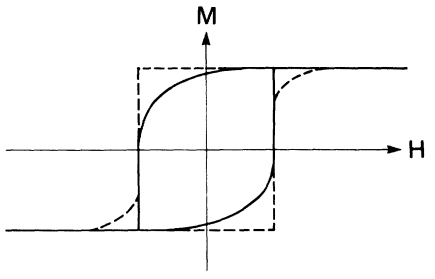

FIG. 1. Typical surface (solid line) and bulk (dashed line) magnetization curves when the magnetic field H is applied in the easy direction of the bulk. M is the magnetization.

The magnetization M_S of the surface sheet tends to lie along the easy direction determined by K_S. If the direction of K_S differs from the easy direction of the bulk, the exchange coupling across the surface-bulk interface will act on the first-layer magnetization M_{1B} of the bulk and may force it out of its own easy direction thereby creating the tail of a domain wall. There is an energy associated with the formation of such fractional domain walls that depends on the bulk exchange stiffness A, the bulk anisotropy K, and on the strength of the external field H. For the calculation of surface-hysteresis loops, one needs to know this energy as it represents the barrier which determines whether M_S can have a direction different from the direction of M_B. Inspection of Fig. 1 indicates that M_S does indeed deviate from M_B particularly if H approaches H_C, but it is also obvious that a long tail of a domain wall does not exist as bulk loops are observed after a few layers distance from the surface.

II. TAILS OF DOMAIN WALLS IN EXTERNAL MAGNETIC FIELDS

Zijlstra[13] calculated the energy of a tail of a domain wall in an external field for a uniaxial material with exchange stiffness A and anisotropy K. If ψ is the angle by which the first bulk layer magnetization M_{1B} deviates from the easy direction of the bulk along which H is applied, one obtains for the energy $\gamma'(\psi,h')$ of the tail of a domain wall per unit area

$$\gamma'(\psi,h')=2\sqrt{AK}\int_0^{\psi}(1-\cos^2\phi-2h'\cos\phi+2h')^{1/2}d\phi\ , \tag{1}$$

where $h'=H/H_A$, with $H_A=2K/M$ being the anisotropy field. Equation (1) has a very simple solution if ψ is small, i.e., if $\cos\phi=1-\phi^2/2$, namely

$$\gamma'(\psi,h')=2\sqrt{AK}\,(1-\cos\psi)(1+h')^{1/2}\ . \tag{2}$$

We see that $\gamma'(\pi,0)$ generates the familiar $4\sqrt{AK}$ which is the energy of a 180° domain wall in uniaxial material. The main obstacle to applying Eq. (2) to the present case of Fe resides in the old dilemma of the theory that $H_C \neq H_A$. This arises because Eq. (1) is derived on the rotation model in which it is assumed that the external field provides the energy to build a domain wall and thus overcomes the barrier to magnetization reversal. In reality, Fe and most magnetic materials switch the magnetization at $H=H_C \ll H_A$. The explanation of

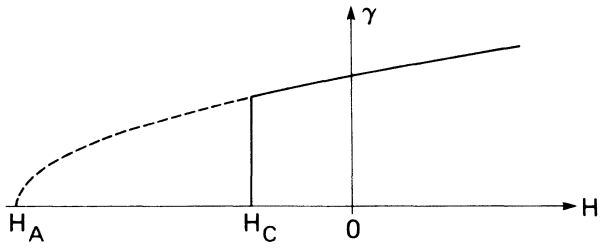

FIG. 2. The energy per unit area γ of a tail of a domain wall vs applied field H. The dashed line is γ' from Eq. (2) derived on the rotation model for small tails. H_C is the coercive and H_A the anisotropy field.

this phenomenon, frequently referred to as Brown's paradox, is probably due to preexisting embryonic domain walls that can be torn free from pinning defects and travel through the material thus reversing the magnetization at much lower external fields.[14] In Fe, $H_A=634$ Oe, whereas $H_C=10$ Oe with the specific crystal considered here.[9] The realistic energy of the tail of a domain wall is shown in Fig. 2. It should be γ' for $H>H_C$, but decrease abruptly as $H\rightarrow H_C$. With

$$\gamma(\psi,h)=2\sqrt{AK}\,(1-\cos\psi)(1+h)^{1/n} \tag{3}$$

and $h=H/H_C$ we can approximate the curve shown in Fig. 2 if n is chosen appropriately. The deviation of the energy γ in Eq. 3 from the ideal energy is given to first order by $(\gamma-\gamma')/\gamma=(H_C/2H_A-1/n)h$ for $-1<h<+1$. Therefore, the best choice of n depends on H_C/H_A; with $H_C=H_A$, for instance, $n=2$ as expected, but for $H_C\ll H_A$ as in the case of Fe, n has to be large. However, already with $n=10$, γ in Eq. (3) deviates by less than 9% from the ideal wall energy in the range of h values that are of interest for calculating hysteresis loops.

III. CALCULATION OF SURFACE-HYSTERESIS LOOPS

With Eq. (3) we can now write the magnetic part δ of the surface energy per unit area in units of the wall energy constant $\sqrt{AK}$:

$$\delta=2(h+1)^{1/n}(1-\cos\psi)+\lambda[1-\cos(\theta-\psi)]$$
$$+\mu\sin^2(\theta-\theta_0)+2\kappa h(1-\cos\theta)\ . \tag{4}$$

θ and ψ are the angles between the external field h and the surface magnetization M_S and the first layer bulk magnetization M_{1B}, respectively. The magnetic field $h=H/H_C$ is applied along the easy direction in the bulk and is measured in units of the bulk coercivity H_C. The first term is the energy of the tail of a domain wall $\gamma/\sqrt{AK}$ from Eq. (3). The last three terms are the familiar energy of the exchange coupling between surface and bulk, the anisotropy, and the field energy of the surface sheet, respectively. The dimensionless parameters are given by the following expressions: $\kappa=H_CM_Sd/(2\sqrt{AK})$ and $\lambda=A_{1,2}/(d\sqrt{AK})$ with $A_{1,2}$ the exchange stiffness between surface and bulk on a path perpendicular to the surface and $\mu=K_Sd/\sqrt{AK}$. Further, d is the thickness of the magnetically different sheet at the surface, θ_0 the angle of the easy direction of the surface magnetization with the external magnetic field, and K_S the strength of the surface anisotropy. One now has to determine values for the parameters κ, λ, μ, and θ_0, and then find the angles θ' and ψ' for which δ is at minimum by computation. The relative surface magnetization is obtained as $\cos\theta'$ and can be compared to the experimental relative spin polarization $\mathbf{P}(h)/\mathbf{P}(\infty)$. The first layer relative bulk magnetization is also obtained from $\cos\psi'$ and has to agree with the experimental data as well.

It is relatively easy to gain insight into the physical meaning of Eq. (4) if $\psi\simeq 0$ or $\simeq\pi$ as suggested by the experiments in the case of the Fe(100) surface. Confining the interpretation to $|h|<1$ which yields $(1+h)^{1/n}\simeq 1$, and omitting terms independent of θ one obtains from Eq. (4).

$$\delta'=\mu\sin^2(\theta-\theta_0)-2\kappa(h\pm\lambda/2\kappa)\cos\theta\ . \tag{5}$$

From the pioneering work of Stoner and Wohlfarth,[15] it is well known that Eq. (5) delivers the hysteresis loop of a uniaxial ferromagnet in an external field h, however, the loop will be shifted on the h axis by $\pm\lambda/2\kappa$ depending on the magnetization direction in the underlying bulk. If we assume $\theta_0=90°$, that is if the easy direction of the surface is perpendicular to the one in the bulk, we obtain a straight line magnetization curve of slope κ/μ shifted by $\pm\lambda/2\kappa$. From the experimental observation that the surface loop changes at $|h|\lesssim 1$ it is inferred that κ/μ as well as $\lambda/2\kappa$ are of the order of unity. This shows that in order to obtain the actual values of μ and λ by fitting calculated hysteresis loops to experiment one has to know the value of the parameter κ. Since $\kappa=H_CM_Sd/(2\sqrt{AK})$, it may be calculated from the values of A, K, and H_C as obtained from conventional bulk measurements; M_S and the thickness d of the surface sheet have to be estimated. Present knowledge on the magnetic probing depth of secondary electrons suggests, as pointed out above, that d should be of the order of the lattice parameter of bcc Fe which is 0.286 nm. M_S cannot be vastly different from the bulk magnetization of Fe which is 2.1 T at $T=0$; It has been suggested[4] that M_S might be larger at $T=0$, yet it is known that thermal excitations will cause a noticeable decrease of M_S even at room temperature where the experiments[9] have been done. With $H_C=10$ Oe, $\sqrt{AK}=0.66$ J/m^2, $M_S=2.1$ T, and $d=0.3$ nm one obtains $\kappa=2.5\times10^{-4}$. This estimate of κ could be in error by 50% but not by much more.

Figures 3(a) and 3(b) show surface-hysteresis loops calculated from Eq. (4) with the assumption $\kappa=2.5\times10^{-4}$ and compares them to the experimental observations. The data point from Ref. 9 exhibit a small drift of the zero of the electron spin polarimeter as the hysteresis loop is not closed when H sweeps from $+30$ to -30 Oe and back to $+30$ Oe. This drift has been eliminated with the assumption that it was linear in time. The best fit to the data is obtained in Fig. 3(a) with $\theta_0=75°$, $\mu=2\times10^{-4}$, $\lambda=4.6\times10^{-4}$. Figure 3(b) shows, however, that $\theta_0=90°$, $\mu=5\times10^{-4}$, and $\lambda=9\times10^{-4}$ also lead to an acceptable, yet clearly somewhat poorer interpretation

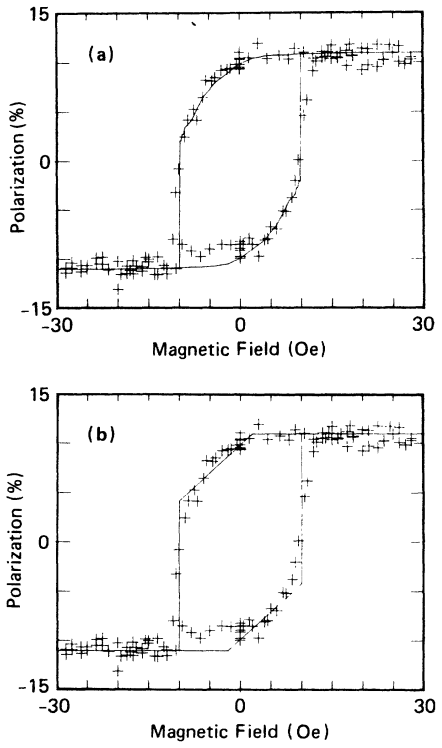

FIG. 3. (a) Surface-hysteresis loop with the Fe(100) surface at room temperature. Crosses are the experimental values of the electron-spin polarization in percent measured with secondary electrons at an energy of 50 eV excited by unpolarized primary electrons of 100 eV from Ref. 9. The solid curve is calculated from Eq. (4) with $n=10$, $\kappa=2.5\times10^{-4}$, $\lambda=4.6\times10^{-4}$, $\mu=2\times10^{-4}$, and $\theta_0=75°$. The fine structure in the calculated curve has no physical meaning as it depends on the size of the angular net used in the calculation. (b) Same as (a) but the solid line is calculated with $n=10$, $\kappa=2.5\times10^{-4}$, $\lambda=9\times10^{-4}$, $\mu=5\times10^{-4}$, and $\theta_0=90°$.

of the experiment. $\theta_0=45°$ can be excluded as the magnetization drops too steeply when $\mathbf{h}\rightarrow-1$. However, a surface with an inhomogeneous direction of the magnetic anisotropy can reproduce the available data very well too; for example, a mixture of two types of patches with $\theta_0=45°$ and $\theta_0=90°$ cannot be distinguished from a homogeneous surface with $\theta_0=75°$.

Clearly, the experiment suggests $\lambda\ll1$. It follows that $\psi\simeq0$ or $\simeq\pi$. Hence, the small values of λ obtained from the experiment automatically lead to square loops for the first bulk-layer magnetization M_{1B} in gratifying agreement with the observation. Therefore, the model not only reproduces the surface loops very well, but also delivers an explanation for the observed strikingly fast change to square bulk loops on increasing the magnetic probing depth. There are two additional independent verifications of the applicability of Eq. (5) or rather (4). Allenspach *et al.*[9] also measured the virgin magnetization curve. The initial slope of this curve turned out to be equal to the slope of the hysteresis loop at $0\geq h>-1$ as noted already before.[16] This can readily be derived from Eq. (5) for $\theta_0=90°$, since the slope of the magnetization curve is constant and equal to μ/κ. In the demagnetized state, $\lambda=0$ on the average and the slope of the unshifted, virgin curve and the curves shifted by $\pm\lambda/2\kappa$ must be identical. Furthermore, Allenspach *et al.*[9] found that the surface-hysteresis loop was reversible for $-0.8\leq h\leq0$. The magnetization curves described by Eq. (5) also show no hysteresis for the above range of h if $\theta_0\geq45°$.

IV. DISCUSSION OF THE RESULTS AND CONCLUSIONS

The numerical values obtained for λ and μ depend on the rather simple assumption that only one sheet at the surface is different from the bulk. It is therefore only the order of magnitude of these parameters that is amenable to a meaningful physical interpretation. From

$$\lambda=A_{1,2}(d\sqrt{AK})=(A_{1,2}/A)(\sqrt{A/K}/d)\simeq5\times10^{-4},$$

we obtain the exchange stiffness $A_{1,2}$ along a path perpendicular to the surface in units of the spherically averaged value of A in the bulk. The thickness of a domain wall in Fe is $\sqrt{A/K}=12$ nm. Hence, we see that $A_{1,2}$ is reduced by 10^{-5} compared to A. However, it is known from the experiments with epitaxial Fe(100) that the exchange coupling within one layer is strong, leading to ferromagnetic order with T_C near room temperature and higher as soon as one layer or more is deposited.[2,3] This large exchange coupling of atoms in the plane of the surface is needed to understand the surface-hysteresis loops; if the exchange was not high within the surface sheet, and the coupling to the bulk as weak as found here, one would observe paramagnetism at the surface of Fe(100) at room temperature.

The weak coupling of the surface sheet to the bulk cannot directly be interpreted as there are no reliable first-principles calculations of exchange interactions. The present dramatic alteration of the exchange at the surface is a surprising, yet not a unique, result. For instance, Weller *et al.*[17] reported that the first layer of the Gd(1000) surface is coupled antiferromagnetically to the bulk although ordering ferromagnetically within the layer; furthermore, it is still ferromagnetic at 22 K above the Curie temperature of the bulk.[18]

One further observation with the Fe(100) surface sheds additional light on the weak bulk-to-surface coupling. The surface loops showed rounded edges as defined in Fig. 1 at all energies of the secondary electrons when the surface was not annealed and recrystallized after argon bombardment.[9] This indicates that the thickness d of the weakly coupled surface sheet must have increased on introducing crystalline disorder. Based on evidence derived from magnetic bulk properties of amorphous Fe-alloys it is known that disordered Fe is weakly coupled, due to the antiferromagnetic contributions of the Fe-atoms at smaller distances.[19] Hence, disorder caused by argon bombardment is expected to reduce the exchange interaction, yet at a different depth, in agreement with the observation. Pierce and coworkers[11] noted similar effects of Ar bombardment and annealing on the surface hysteresis loops of FeB glasses; incorporation of Ar may also be an element to be considered in the interpretation of these

data.

Essential for the detection of the weak surface-to-bulk exchange is the change in the easy direction of magnetization at the surface by the angle θ_0. From $\mu = K_S d/\sqrt{AK} = (K_S/K)(d/\sqrt{A/K})$ we obtain the strength of the surface anisotropy K_S in units of the bulk anisotropy K. It is $K_S \simeq 10^{-2}K$. With $\theta_0 = 90°$, this weak anisotropy could be due to magnetostrictive stress created by the underlying bulk. Alternatively, one might consider whether it could be due to textures created in the process of sputter cleaning. For $\theta_0 = 75°$ or a mixture of $\theta_0 = 45°$ and $= 90°$ patches, the explanation of K_S most likely involves atoms located at special surface sites like steps. Changes in the direction of the surface anisotropy have also been reported by Korecky and Gradmann[19] who found that the easy direction of magnetization is (110) instead of (100) at the Fe(110) surface.

The perpendicular anisotropy found at the surface of epitaxial Fe(100) films should also be considered as a possible explanation for the difference between bulk and surface anisotropy. We believe, however, that this is unlikely to apply for the following reasons. Generally, the anisotropy of a film magnetized perpendicular to the surface is given by $K_S = M_S{}^2/2\mu_0 - K_S^i$ where K_S^i is the intrinsic anisotropy. If $K_S^i > M_S^2/2\mu_0$, the easy direction of magnetization is perpendicular to the surface. According to Refs. 1 and 2 spontaneous perpendicular magnetization is observed in epitaxial Fe films of 2–5 layers at $T < 70$ K. The magnitude of $M_S/2\mu_0$ is $\simeq 21.5$ kOe and of $K_S^i \simeq 22$ kOe. At $T > 100$ K, M_S lies in plane indicating that now $K_S^i < M_S^2/2\mu_0$. The small value of $\mu = 10^{-4}$ obtained for the (100) surface of bulk Fe would then indicate that $M_S^2/2\mu_0$ and K_S^i happen to compensate each other to an accuracy of one part in 10^3 at room temperature which is indeed unlikely. Without any doubt, it is conceivable that the vector of the surface magnetization M_S encloses an angle $\alpha \neq 90°$ with the surface normal due to additional perpendicular anisotropies at least at certain temperatures as proposed in Ref. 7. The relatively low value of the saturation spin polarization of only 11% in the plane of the surface (compare Fig. 3) could be due in part to such a phenomenon, as the saturation polarization of large-probing-depth secondary electrons was found to be 27%.[9] Although α could be $\neq 90°$, it is unlikely to change on applying fields as low as the coercive field of 10 Oe. The changes of the direction of M_S observed in the very-low-field regime are thus most likely due to rotation of M_S around the surface normal at $\alpha = \text{const}$. It is clear that further experiments with very strong magnetic fields applied perpendicular to the surface are needed to clarify the question of whether $\alpha \neq 90°$ at the Fe(100) surface.

The most important implication of the weak perpendicular exchange at the Fe(100) surface concerns the temperature dependence of the surface magnetization. The decrease of the spontaneous magnetization at low T is caused by thermal excitations of spin waves. Bloch showed that the relative magnetization of the bulk decreases according to $M(T)/M(0) = 1 - C_B T^{3/2}$. Rado[20] noted that all waves have an antinode at the surface and that M_S should therefore decrease like the bulk with $T^{3/2}$, but the prefactor should be $2C_B$. However, for the Fe(110) surface[21] and for the surface of $Fe_{40}Ni_{40}B_{20}$,[22] it was found that the prefactor is $3C_B$. Mathon[23] showed that this stronger thermal decrease of the surface magnetization can be understood with the assumption that the exchange interaction on a path perpendicular to the surface is weakened. We find from very different experimental evidence that the perpendicular exchange interaction is practically zero at the surface of Fe (100), whereas ferromagnetic order exists within the plane of the surface sheet. This is not a contradiction to the general result that ferromagnetic order cannot exist in two-dimensional structures.[24] Namely, the existing exchange coupling to the bulk produces an effective magnetic field in the surface as shown above which can stabilize the ferromagnetic state of the surface layer. We believe that the considerations put forward by Mathon and Ahmad[25] for the case of weak perpendicular exchange apply to the case of the Fe(100) surface. The temperature dependence of M_S will then be totally different from expectations based on the usual assumption of bulklike exchange coupling constants.

Generally, surfaces and interfaces are known to play a decisive role in determining coercivity and wall pinning, and therefore, it is to be expected that exchange stiffness and anisotropy near surfaces will play a major role in applied magnetism as well. In the case of Fe(100), the very surface turns out to be weakly coupled to the bulk so that the magnetic properties of the first layer can exercise no major influence on magnetic coercivity and domain wall pinning at the surface. This could be an exceptional case as only very rudimentary experience exists concerning these properties at other surfaces of Fe and other materials. However, the actual value of the weak surface-to-bulk exchange coupling as well as that of the small surface anisotropy would not have been anticipated before we determined them. As we have shown, these small values are consistent with a large body of experimental observations. The fundamental explanation of the values that we have established for the surface to bulk exchange coupling and the anisotropy of Fe(100) is a challenge for electronic structure theorists.

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