Magnetization and susceptibility of ultrathin Fe films on Cu(100)

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Face-centered Fe on Cu(100) remains a challenging and rich magnetic film system due to its structural and magnetic instabilities. One magnetic phase has a spin structure where the first two layers are coupled ferromagnetically and the remaining layers are all antiferromagnetically coupled. We use a self-consistent local mean-field method, to calculate the magnetic structure of this phase for any temperature and applied field. We obtain theoretical results for both parallel and transverse susceptibility measurements and indicate how such measurements may be used to determine the anisotropy in the ferromagnet and antiferromagnet portions of the Fe film. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1359470]

At room temperature, bulk Fe normally has a bcc structure. In contrast, fcc Fe is normally a high-temperature phase. However, face-centered phases of Fe can be stabilized via epitaxial growth on a fcc substrate such as Cu(100). These structures are influenced by many factors such as lattice mismatch, growth energetics, film morphology, interdiffusion, etc., to form subtly different, metastable face-centered phases.[1–5]

In this article we explore theoretically the magnetic properties of one of the most interesting magnetic structures of fcc Fe. For the films grown above ~250 K and with thicknesses of 6–11 monolayers (ML), one finds ferromagnetic coupling between the top two ML and antiferromagnetic coupling for the remaining layers. Ferromagnetic ordering is observed at the surface below 260 K while the antiferromagnet (AF) ordering apparently disappears around 175–200 K.

We now present a theoretical calculation for the magnetic structure of Fe on Cu(100) and explore the influence of anisotropy (previously neglected) on the magnetic results. It is clear that there is some kind of anisotropy in the system as the experimental data[6] at low temperatures showed a coercivity of about 300 G. Our theoretical calculations are based on a self-consistent local mean field theory.[7] This method has been applied in a number of systems and has given a good description of both the temperature and field behavior of magnetic layered structures.[8–10]

We use a Heisenberg-type Hamiltonian for the system that uses an effective exchange coupling between spins S_i in layer i and S_{i+1} in the neighboring layer. Only couplings between nearest neighbor layers are included. A small external field, H_0, and an anisotropy field, H_a, are also included. The uniaxial anisotropy has the direction normal to the surface as the easy axis. Thus,

$$H=-\sum_{\text{layer } i} A_{i,i+1}\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \sum_{\text{layer } i} g\mu_B\mathbf{H}_0\cdot\mathbf{S}_i - \sum_{\text{layer } i} g\mu_B\mathbf{H}_a(\mathbf{S}_i^{(z)}/S_{\max})\cdot\mathbf{S}_i^{(z)}.$$

The parameters used are $S=1$ and $g=2.2$. The exchange coupling constants are given in terms of temperature. The ferromagnetic coupling between the first two layers is found to be $A_{1,2}/k_B=360$ K while the antiferromagnetic coupling between all other layers is taken as $A_{i,i+1}/k_B=-130$ K. To put these values into perspective, the ferromagnetic exchange coupling for bulk (bcc) Fe is about 530 K. Our choice of parameters was based initially on the experimentally observed values of T_N and T_C but these were modified by finite size effects. For example, for the ferromagnet the Curie temperature would indicate an exchange constant of $A/k_B=193$ K for a bulk sample. Because of finite size effects we need to use an increased value of $A/k_B=360$ K.

We note that a similar model has been used recently[11] to explain some interesting features of the experimental data for ultrathin fcc Fe on Cu(100). In particular, the magneto-optic-Kerr-effect data showed a puzzling linear behavior of $\Delta M(T)$, the temperature dependence of the oscillation in the magnetization as a function of thickness occurs because $\Delta M(T)$ measures the temperature dependence of the outermost layer of spins. The theory also showed that $M(T)$ for the eleven layer structure should decrease at low temperature in agreement with experiment.

An iterative method is used to find the ground state for the Hamiltonian as a function of temperature and applied field. Figure 1 explores the susceptibility as a function of temperature when the applied field and ΔM are perpendicular to the surface. Here and below we calculate this susceptibility numerically, i.e., $\chi=[M(H_0+\Delta H)-M(H_0)]/\Delta H$. It is not exactly clear what one should expect. Normally one finds peaks in susceptibility near phase transitions. In this case, however, the phase transition associated with the vanishing of the antiferromagnetic order (175–200 K) is smeared out due to finite size effects. This results in a broad peak rather than a sharp peak. Furthermore, the AF contribution to the susceptibility is simply much smaller than the ferromagnet contribution and as a result one only sees a sharp peak corresponding to the ferromagnetic phase transition near $T=260$ K.

Figure 2 examines a different susceptibility. Here the applied field and ΔM are parallel to the surface. There is a broad peak at temperatures around 180–250 K. In contrast to

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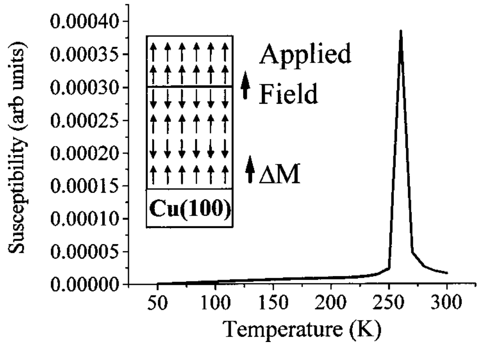

FIG. 1. Susceptibility as a function of temperature when the applied field and ΔM are perpendicular to the surface. $H_a = 20$ G in both the ferromagnet and antiferromagnet. The inset shows a schematic of the measurement. $H_0 = 2$ G and $\Delta H = 0.1$ G. The ten and eleven layer structures give essentially the same results.

Fig. 1, the peak in this figure does not arise from a thermal phase transition, but is caused instead by a magnetic reorientation. The shape and position of the peak depends on the strength of the applied field. At low fields and temperatures the spins are all nearly perpendicular to the surface since the external field does not overcome the anisotropy. As the temperature is increased, however, the effective anisotropy field $H_a \langle S^{(z)} \rangle / S_{\max}$ is reduced in magnitude and the spins rotate from normal to the surface to something where the moments have a component parallel to the surface. The large values of susceptibility occur when large changes in the spin configuration can occur. For larger external fields the applied field can overcome the effective anisotropy field at lower temperatures so we see a peak near 190 K, for example, when $H_0 = 20$ G. If the applied field is smaller than larger temperatures are needed to reduce the anisotropy field and allow rotation of the spins. As a result the peak in the susceptibility occurs at higher temperatures. For the smallest applied field we see both a broad peak associated with the reorientation and a sharp peak associated with the thermal phase transition.

We now examine the question of whether one can learn if the anisotropy is in the ferromagnetic layers or in the antiferromagnetic layers. In Fig. 3 we again see a susceptibility defined when the applied field and ΔM are parallel to the surface. We consider the case where $H_0 < H_a$ so that the orientation of the spins at low temperature is essentially normal to the surface. The top curves are for the case that the only anisotropy is in the ferromagnet and the bottom set of curves show results when the anisotropy is in the antiferromagnet. We see the ferromagnetic results involve long plateaus at low temperatures and rapid drops near the ferromagnetic transition temperature $T = 260$ K. In contrast, the

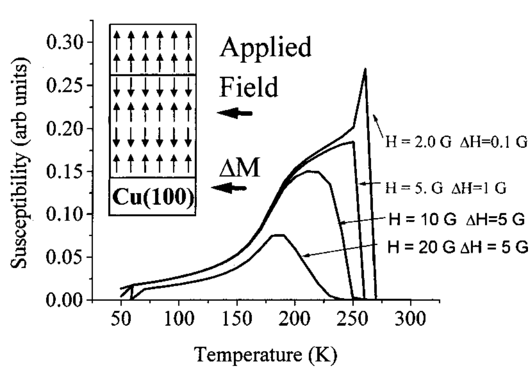

FIG. 2. Susceptibility for the case when the applied field and ΔM are parallel to the surface. The peaks are not due to thermal phase transitions but are instead caused by a spin reorientation. The structure has eleven layers (two F and nine AF) and $H_a = 20$ G in both the ferromagnet and antiferromagnet.

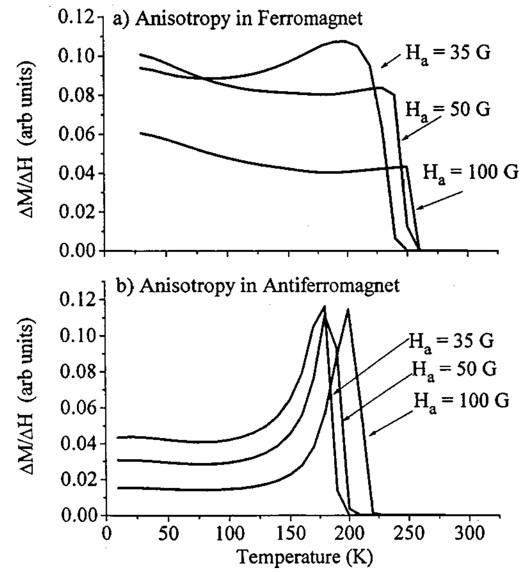

FIG. 3. Susceptibility for the case when the applied field and ΔM are parallel to the surface. The applied field is 20 G and $\Delta H = 5$ G. The calculation is for a ten layer structure (two F layers and eight AF layers.) In (a) the uniaxial anisotropy is located in the ferromagnet only while in (b) it is in the antiferromagnet.

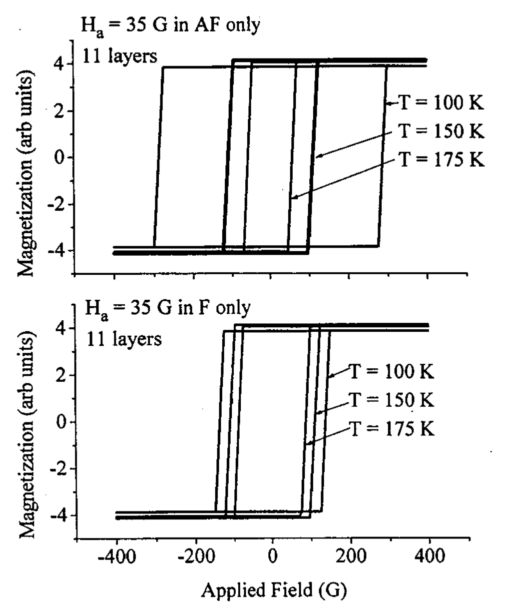

FIG. 4. Hysteresis curves for an eleven layer structure (two F layers and eight AF layers) at different temperatures. The applied field is 20 G and $\Delta H = 5$ G. When the anisotropy is in the antiferromagnetic layers there is a large change in coercive field as the temperature changes.

systems with anisotropy in the antiferromagnet show plateaus at low temperatures followed by rapid increases and then rapidly drops near the antiferromagnetic transition of $T=200$ K. This different behavior should allow determination of the location of the anisotropy in this coupled system.

Figure 4 investigates a different method to determine the location of the anisotropy. Here we present the calculated hysteresis curves for an eleven layer structure (two F layers and nine AF layers) at different temperatures. The top set of curves show the results if the anisotropy is in the antiferromagnet, while the lower curves show the results for the case where the anisotropy is in the ferromagnet. It is immediately obvious that the coercive field has a much stronger temperature dependence if the anisotropy is in the antiferromagnet. This is to be expected since the antiferromagnet has a lower transition temperature and thus the thermal anisotropy field, $H_a\langle S^{(z)}\rangle/S_{\max}$, changes substantially from 100 to 175 K. This results, in turn, in a large change in the coercive field. The results for a ten layer structure (two F layers and eight AF layers) are qualitatively similar.

In summary we have calculated the magnetic structure for a phase of fcc Fe on Cu(100) using a self-consistent local mean-field method. This phase is characterized by two ferromagnetic layers at the surface and the remaining layers are all antiferromagnetically coupled. We include anisotropy in the Hamiltonian and show that the temperature dependence of the susceptibility can show whether the anisotropy is primarily in the ferromagnet or the antiferromagnet. Furthermore, we show that a rapid variation in coercive field with temperature indicates that the anisotropy is located primarily in the antiferromagnet.

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[1] J. Thomassen, Phys. Rev. Lett. **69**, 3831 (1992).
[2] S. Müller *et al.*, Phys. Rev. Lett. **74**, 765 (1995).
[3] M. Zharnikov *et al.*, Phys. Rev. Lett. **76**, 4620 (1996).
[4] J. Shen *et al.*, Europhys. Lett. **43**, 349 (1998).
[5] H. Magnan *et al.*, Phys. Rev. Lett. **67**, 859 (1991).
[6] D. Li *et al.*, Phys. Rev. Lett. **72**, 3112 (1994).
[7] R. E. Camley and D. R. Tilley, Phys. Rev. B **37**, 3413 (1988).
[8] R. E. Camley, J. Kwo, M. Hong, and C. L. Chien, Phys. Rev. Lett. **64**, 2703 (1990).
[9] A. S. Carriço and R. E. Camley, Phys. Rev. B **45**, 13 117 (1992).
[10] M. Sajieddine *et al.*, Phys. Rev. B **49**, 8815 (1994).
[11] R. E. Camley and D. Li, Phys. Rev. Lett. **84**, 4709 (2000).