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Magnetic anisotropy of epitaxial Fe films grown on curved W(001) with a graded step density

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Ultrathin Fe films were grown epitaxially onto a stepped W(001) substrate, polished with a curvature to provide a continuously variable step density, with the steps parallel to the [100] crystalline axis. The steps induce an in-plane uniaxial magnetic anisotropy with easy axis perpendicular to the step edges. We found that this step-induced magnetic anisotropy does not enhance the Curie temperature of the Fe film. The strength of the anisotropy varies quadratically with step density, but does not decay with $1/d$ dependence expected for a surface-type anisotropy. We suggest that strain at the step edges might underlie the result. [S0163-1829(98)50620-0]

Interest in low-dimensional magnetic systems has intensified in the last decade due to the discoveries of antiferromagnetic coupling[1] and giant magnetoresistance[2] in magnetic multilayers. Thin-film technology has played an essential role due to the ability to control thickness on the monolayer (ML) scale. Despite the great progress made with layered structures, significantly less effort has been devoted to the lateral confinement of magnetic structures. The technical difficulty derives from the short-range character of the magnetic interactions, which demands a nanometer-scale lateral confinement in order to manifest the quantum nature of the magnetism. In efforts to achieve this goal, several groups have fabricated metallic films on *stepped* surfaces. For example, nanometer-scale Cu wires have been decorated onto atomic step edges of a Mo(110) surface[3] and the steps were shown to modulate macroscopic magnetic properties.[4–7] One of the magnetic properties studied recently is the magnetocrystalline anisotropy, which originates from the spin-orbit interaction,[8] and hence is sensitive to the symmetry of the lattice. Atomic steps can locally break the rotational symmetry of the surface of an oriented single crystal and induce a uniaxial anisotropy within the film plane. This kind of step-induced anisotropy has been observed in several magnetic overlayer systems grown on stepped substrates, such as Co/Cu(100),[4,5] Fe/W(100),[6] and Fe/Ag(100).[7] To explore the role of symmetry breaking in the step-induced anisotropy, Kawakami, Escorcia-Aparicio, and Qiu[7] investigated Fe films on a *curved* Ag(001) substrate. They found a quadratic relation between the step-induced anisotropy and the step density,[7] and proposed a simple explanation based on Néel's pair-bonding model.[9] They omit, however, the effect due to the lattice misfit of 42.5% in the vertical direction and 0.77% in the lateral direction between the bcc Fe and the fcc Ag. Another important consequence of Néel's model is a $1/d$ dependence of the step-induced anisotropy, where d is the film thickness. Weber *et al.*, however, observed an oscillatory behavior in the strength of the step-induced anisotropy upon increasing the film thickness in a Co/Cu(100) system.[5] To understand the origin of the step-induced magnetic anisotropy, more research is needed to probe different lattice symmetries with different lattice misfit. To that end, we report in this paper, results for the Fe/W(001) system, where both Fe and W are bcc and have a lattice misfit of $(a_W - a_{Fe})/a_{Fe} = 10.1\%$ in both directions, which contrasts with that of the Fe/Ag case. We find that the step-induced anisotropy depends quadratically on the step density, but is only weakly thickness dependent, suggesting that its origin is not *surface* based, but might be *strain* related. Moreover, we find that this step-induced magnetic anisotropy has no effect on the Curie temperature of the Fe film.

A W(001) single-crystal disk 2 mm thick and 10 mm in diameter was mechanically polished down to a 0.25-μm diamond-paste finish. The (001) orientation was preserved over half the surface, while the other half was polished to form a curved shape with a vicinal angle ranging from 0° to 9° to provide a continuous variation in the step density. The step edges are parallel to the [100] axis of the crystal. The W substrate was ultrasonically cleaned in acetone before being put into an ultra-high-vacuum chamber of base pressure $\sim 7\times10^{-11}$ Torr. The substrate was mounted on a sample manipulator by a W wire (1-mm diameter by 10-cm length) and heated via electron bombardment. The heater was a 0.25-mm diameter W filament located ~ 5 mm behind the sample. By applying $+1.5-1.7$ kV to the substrate and $\sim 6-7$ A to the filament, the W crystal could be heated to 2300 °C. The substrate was cleaned by cycles of annealing at 1500 °C in $\sim 10^{-7}$ Torr O_2 for $\sim 5-15$ min and flashing to ~ 2300 °C in the absence of O_2. This is a standard cleaning method for W surfaces.[10–12] The growth of Fe on W(001) has been extensively studied in the literature.[13–15] Fe films were grown onto the W substrate at room temperature using a water-cooled evaporator. Fe wedges also were fabricated; this was achieved by moving the substrate behind a knife-edge shutter during the deposition. The deposition rate was ~ 0.5 Å/min, and the slope of the wedges was ~ 0.5 Å/mm. The pressure during the growth was $\sim 3-5\times10^{-10}$ Torr.

Surface magneto-optical Kerr effect (SMOKE) measurements were taken at room temperature with a He-Ne laser light source focused at different positions along the curved substrate. As the laser beam scans across the sample to mea-

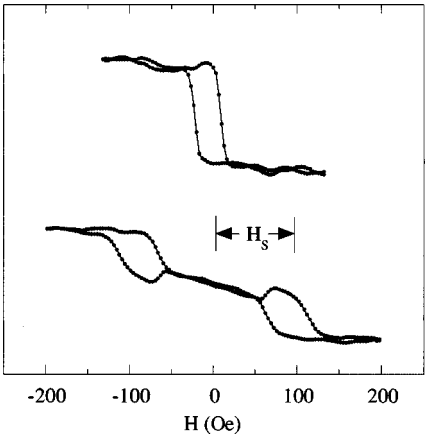

FIG. 1. Hysteresis loops for a 2-ML Fe film grown on a 4.7°-miscut stepped W(001) surface. The square loop is for H perpendicular to the step edges and the split loop is for H parallel to the step edges. This indicates the presence of a uniaxial magnetic anisotropy with easy axis perpendicular to the step edges.

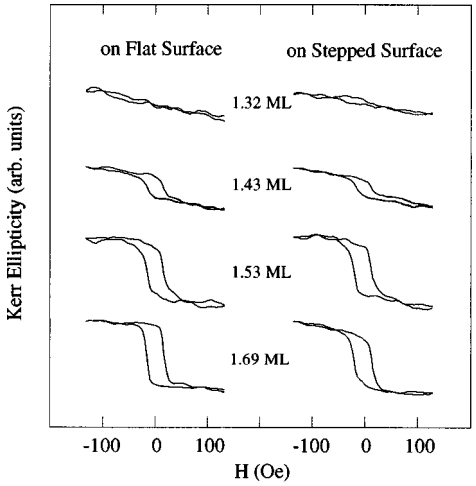

FIG. 2. Easy-axis hysteresis loops at room temperature for Fe films grown on flat and 4.7°-miscut stepped W(001) surfaces. No enhancement of the Curie temperature on the stepped surface is observed.

sure hysteresis loops, the reflection angle of the beam simultaneously determines the local vicinal angle. The beam size of ~ 0.3 mm would cover $\sim 0.7°$ of vicinal angle, but a narrow slit was placed on the reflection path to improve the angular resolution to $\sim 0.2°$. The magnetization is in the film plane, thus only longitudinal hysteresis loops are reported herein; no polar SMOKE loops were observed.

Figure 1 displays hysteresis loops scaled to a unit saturation magnetization for a 2-ML Fe film on a stepped surface of 4.7° vicinal angle. The loops are square and exhibit full remanence for the magnetic field H applied *perpendicular* to the step edges, but are split and lack remanence for H applied *parallel* to the step edges. This behavior clearly establishes the existence of a uniaxial in-plane magnetic anisotropy with easy axis perpendicular to the step edges. There have been reports in the literature that uniaxial anisotropy is produced by growing sample at an angle. However, our samples were grown at normal incidence, therefore a nonnormal deposition angle as a cause for the uniaxial anisotropy can safely be disregarded. The dips in the split loops are due to the polarization effect of the incident beam,[6] and will be discussed in detail in a subsequent paper. It is interesting to note that the easy axis of magnetization is different from that for the Fe/stepped-Ag(001) and Co/stepped-Cu(001) systems, for which it is parallel to the step edges. This may be due to the differences in the film-substrate electronic hybridization. To explore the possible consequence of step-induced magnetic anisotropy on magnetic properties, we examined the Curie temperatures T_C of the Fe films. First, we can estimate the uniaxial anisotropy due to strain at the steps and the bulk anisotropy with strain using Néel's pair-bonding model. We obtain the same order of magnitude (10^6 erg/cm^3) for both quantities.[22] Figure 2 shows easy-axis hysteresis loops normalized by film thickness for several Fe thicknesses at room temperature. Since it is well known that T_C sensitively scales with the thickness of the ferromagnetic layer (100–200 K/ML), the fact that long-range magnetic orders of the Fe films on the flat and the stepped surfaces disappear at the same thickness, indicates that the step-induced uniaxial magnetic anisotropy does not enhance T_C of the Fe film. This raises an interesting question concerning the origin of the magnetic long-range order (LRO) in the system. It is well known theoretically that an isotropic two-dimensional (2D) Heisenberg system does not exhibit LRO at finite temperature;[16] but adding uniaxial anisotropy stabilizes the LRO and makes the magnetic phase transition Ising-like.[17] While experiments on 2D systems with uniaxial anisotropy support this result, there exist other 2D systems [usually (100) films with in-plane magnetization] whose experimentally determined magnetization critical exponent does not belong to any known universality class.[18] These latter systems could be described more accurately as 2D XY systems possessing bulk magnetic anisotropy. Bulk anisotropy could stabilize the magnetic LRO, but the phase transition should not exhibit universal scaling behavior.[19] Finite-size effects[20] also have been invoked as an alternate explanation of the magnetic LRO and critical exponent of these systems. Thus Fe on stepped W(001) should serve as a good model system here since it evolves from being dominated by a bulk anisotropy when the surface is flat to a uniaxial anisotropy when it is stepped. The thickness independence of T_C suggests that the additional uniaxial anisotropy does *not* alter the magnetic LRO for this 2D XY system with bulk anisotropy. A clearer picture of the nature of the magnetic phase transition might emerge from an experimental study of the critical exponents of the Fe films on the flat and stepped W(001) surfaces.

To better understand the nature of the step-induced anisotropy, the relationship between anisotropy and step density was investigated. Hysteresis loops normalized to a unit saturation magnetization for a 2-ML Fe film are shown in Fig. 3 at different vicinal angles α for H parallel to the step edges (hard axis). The loops are split for $\alpha \neq 0$ and are characterized by a shift field H_s. The system can be described by a step-induced uniaxial magnetic anisotropy K_u and a cubic (bulk) anisotropy term K_1. Thus the energy density is $E = K_u \cos^2 \phi + K_1 \sin^2 \phi \cos^2 \phi - M_s H \cos \phi$, where M_s is the saturation magnetization and ϕ is the angle between the magnetization M and H. This expression has the same form

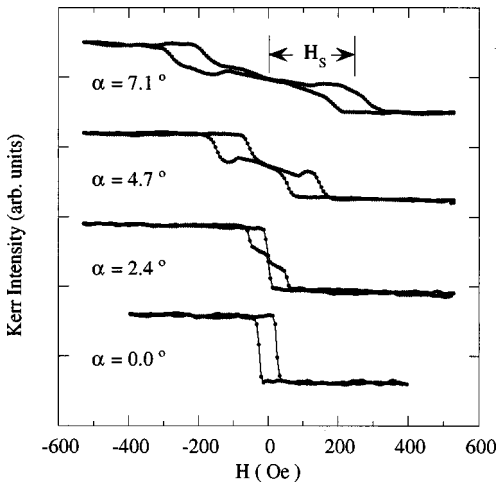

FIG. 3. Hysteresis loops of a 2-ML Fe film on a curved W(001) substrate with H applied parallel to the step edges (hard axis). α is the vicinal angle. The shift field H_s is proportional to the step-induced uniaxial anisotropy.

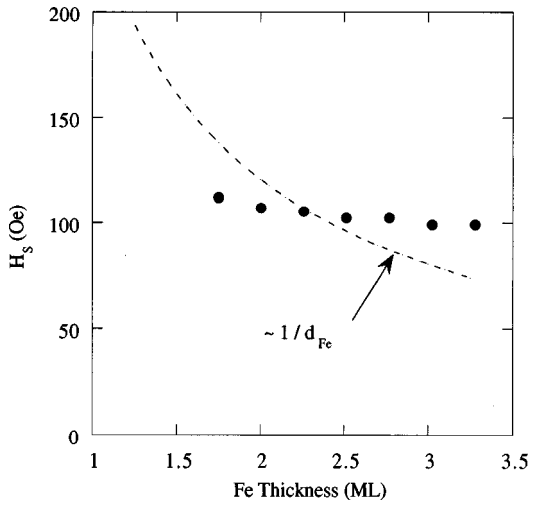

FIG. 5. H_s vs thickness along an Fe wedge, which illustrates the weak thickness dependence as compared to a $1/d$ dependence (dashed curve) expected for a surface-type anisotropy.

as that for an antiferromagnetically coupled sandwich, but with the antiferromagnetic coupling replaced by the uniaxial anisotropy.[21] That is why the hysteresis loops are similar in appearance for the two different types of systems. If the cubic anisotropy is eliminated ($K_1=0$), then M would increase linearly with H and saturates at $H=2K_u/M_s$. A nonzero K_1 opens hysteresis side-loops centered around $|2K_u/M_s|$. Thus, the shift field H_s in Fig. 3 can be used to characterize the strength of the step-induced uniaxial anisotropy. Figure 4 shows H_s vs α measured at different positions along the curved substrate on linear and log-log scales in (a) and (b), respectively. We observe step-induced anisotropy throughout

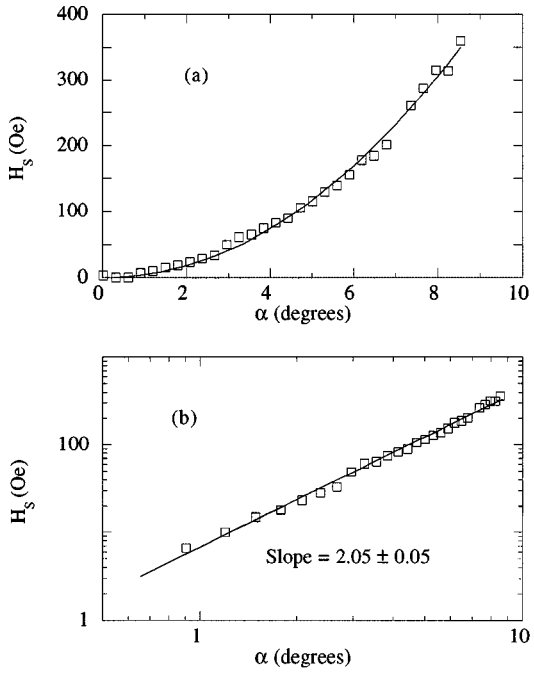

FIG. 4. (a) H_s (from Fig. 3) vs vicinal angle α. The solid line is the result of a power-law fitting, yielding a quadratic relation between H_s and α. (b) Logarithmic plot of H_s vs α, where the quadratic relation is depicted by the straight line.

the 9° angular range studied. (Reference 6 reported that the step-induced anisotropy vanished beyond 6°.) To find the relationship between the step-induced anisotropy and α, we fitted the data to the expression $H_s=A\alpha^n$, with A and n as parameters. The result, $A=4.3\pm0.4$ Oe/degree^n and $n=2.05\pm0.05$, is plotted as the curves in Fig. 4. Thus, the fitting yields a quadratic relation, where the slope of the straight line in Fig. 4(b) gives the power-law exponent $n=2.05$.

The quadratic relation between the step-induced anisotropy and step density raises a question as to the origin of the uniaxial anisotropy. There are several possible explanations. Berger, Linke, and Oepen[4] imaged the magnetic domain structure of the Co/stepped-Cu(001) system and concluded that the observed uniaxial anisotropy cannot be explained by the cubic bulk anisotropy.[4] Dipole-dipole interactions (giving rise to shape anisotropy) might be another candidate for this uniaxial anisotropy. However, one might expect a shape-anisotropy origin to yield a universal direction for the easy axis of magnetization, but the easy axis we observe, perpendicular to the step edges, is opposite to that for the Fe/Ag and Co/Cu systems. Also, Néel's pair-bonding model can result in a uniaxial anisotropy at the step edges.[22] (Recent computer simulations support the idea that step edges can have a strong effect on the coercivity as well.[23]) Kawakami, Escorcia-Aparicio, and Qiu applied Néel's pair-bonding model to a bcc film and found that a coordinate rotation from the crystalline axis to the film axis results in a quadratic dependence of the uniaxial *surface-type* anisotropy on step density.[7] We measured the step-induced anisotropy along an Fe wedge grown on a W(001) substrate with 4.7° vicinal angle, and find only a weak thickness dependence as opposed to the $1/d$ dependence expected for a surface-type anisotropy, as is shown in Fig. 5. We speculate that this could arise from strain induced at the step corners. In Néel's pair-bonding model, each nearest-neighbor bond contributes an anisotropy $K\cos^2\theta$, where K is the anisotropy strength and θ is the angle between the spin and the bond direction. For an atom at the step corner, uniaxial magnetic anisotropy can be generated simply by the reduction of nearest neighbors with-

out the need to change K. This is the effect of lattice symmetry breaking. If there is film/substrate lattice misfit, however, the strain induced at the step corners could result in different anisotropy strength K for different nearest-neighbor bondings. Therefore, the effect of strain at the step corners should be included in the step-induced magnetic anisotropy in addition to the effect of lattice symmetry breaking. Strain due to lattice misfit could persist up to a critical thickness, leading to a volume-type magnetic anisotropy.[24] That is probably why the step-induced anisotropy in the Fe/W system has a very weak thickness dependence. More theoretical work is needed to provide a clear answer.

In the present work, ultrathin Fe films and wedges were grown on a stepped W(001) substrate polished with a curvature to provide a continuous gradation of the step density. The steps induce a uniaxial magnetic anisotropy whose strength depends quadratically on vicinal angle, but the steps do not enhance the Curie temperature. While the origin of the anisotropy is open to discussion, it does not appear to be simply surface-type based, but might be strain induced.

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