Effects of step decoration by oxygen on ultrathin film magnetic anisotropy: $p(1\times1)$Fe on vicinal W(100)

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The mechanisms responsible for surface-step-induced magnetic anisotropy in ultrathin films on vicinal surfaces were explored by studying the effects resulting from surface oxygen adsorption. Magnetic hysteresis loops produced by ultrathin (1–4 ML) Fe films on a variable-step-density W(100) surface were measured using the magneto-optic Kerr effect. Auger electron spectroscopy was used to determine surface oxygen coverage. Significant reductions of the switching fields that characterize the uniaxial surface-step-induced anisotropy were observed. The oxygen-coverage dependencies were found to be consistent with step decoration (preferential chemisorption at steps) and support the highly localized nature of magnetic anisotropy energies associated with the Néel pair-bonding model of surface-step-induced magnetic anisotropy. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1556198]

I. INTRODUCTION

A modified Néel model of surface-step-induced magnetic anisotropy[1] appears to account for vicinal-angle dependencies and remanent magnetization directions of several ultrathin film systems: Fe/W(100),[2,3] Co/Cu(111),[4] Co/Cu(100),[5] and Fe/Ag(100).[6] The Néel model, however, also requires two-dimensional (2D) surface anisotropy behavior (scaling of the anisotropy strength as the inverse of the film thickness), which has not been observed. Recent studies of thicker Fe films (10–60 ML) on vicinal Ag(100) (Ref. 7) found the step anisotropy to be independent of film thickness and unaffected by decoration by Pd atoms. This behavior brings into question the validity of the Néel model in describing surface-step-induced anisotropy, especially in thicker film systems.

The Néel model of surface-step-induced magnetic anisotropy[1] is based on the magnetic pair interaction energy between atoms. Atoms at a surface or at step edges on a vicinal surface experience an environment of reduced symmetry. Missing bonds associated with the broken-symmetry sites are expected to produce new anisotropy energies that will influence magnetic behavior. The highly local nature of the Néel mechanism applied to stepped surfaces, and the known tendency of chemisorbed atoms to migrate to and decorate step sites on a surface, suggest that surface adsorption experiments conducted on ultrathin magnetic film/stepped surface systems may help elucidate the role of the Néel mechanism in determining vicinal surface thin-film magnetic anisotropy.

This article describes oxygen chemisorption experiments that explore the Néel model of vicinal surface ultrathin film magnetic anisotropy. The magneto-optic Kerr effect was used to study hysteresis loops generated by ultrathin (1–4 ML) Fe films on a stepped W(100) surface with continuously varying vicinality (0°–12°) as a function of surface oxygen concentration. Ultrathin Fe films on the stepped surface were found to manifest significant reduction of their characteristic (uniaxial anisotropy) switching fields when exposed to oxygen. The switching field coverage dependence was found to be consistent with step decoration (preferential adsorption at steps at low coverage). At low oxygen coverage (well below 1 ML) films grown on high vicinality surfaces were observed to lose step-induced anisotropy while the same films on low vicinality surfaces retained their anisotropy. This behavior indicates preferred chemisorption at steps and higher sensitivity of step-induced anisotropy due to step decoration than to terrace site chemisorption, which is consistent with general features of the Néel model. The results suggest that a combination of local (Néel-type) anisotropy energy for very thin (<4 ML) films and a nonlocal (magnetoelastic) anisotropy energy that becomes dominant in thicker films is required to generally account for step-induced anisotropy in thin and ultrathin films.

II. EXPERIMENT

The experiments were conducted using an ultra-high-vacuum film growth/characterization chamber described previously.[8] The chamber incorporates pendent-drop electron beam film growth sources, and low energy electron diffraction (LEED) and Auger electron spectroscopy (AES) surface characterization tools. The magneto-optic Kerr effect polarimeter uses a 10 mW HeNe laser and Si photodetectors and operates at a fixed 45° angle of incidence. The drive field is produced by an electromagnet with pole caps inside the

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chamber and coil outside the vacuum system capable of producing 3000 Oe oscillating magnetic fields at low drive frequencies (typically, a few Hz).

The W(100) crystal was prepared to have a flat region [(100) surface normal] and a graded-step-density region in which the vicinal angle, α, varied continuously from zero to approximately 15°. The 1-cm-diam×2-mm-thick crystal was mounted at the tip of a liquid-nitrogen (LN$_2$) dewar that permitted electron beam heating to 2800 °C for cleaning the crystal and the necessary mechanical degrees of freedom for alignment and positioning. Prior to film growth, the W(100) surface was cleaned by standard procedures[2,3] (heating in oxygen to reduce surface carbon followed by flashing to eliminate oxygen). The *in situ* cleaning produced a well-ordered W(100) surface with O and C contamination levels, typically, below 1% of a ML. Similarly, low contamination levels were achieved after the Fe film growth, which was carried out at typical pressures of 4×10^{-10} Torr.

The first layer of $p(1 \times 1)$Fe on W(100) exhibits excellent epitaxy resulting from favorable surface energies of Fe and W, but is nonmagnetic.[2,9,10] Addition of Fe atoms to the monolayer results in a ferromagnetic film that exhibits excellent epitaxy at 2 ML, but begins to manifest strain-relieving dislocations beyond about 3 ML resulting from the lattice mismatch between bcc W ($a = 3.16$ Å) and bcc Fe ($a = 2.86$ Å). Experiments reported in this article cover Fe layer thickness from 1.8 to 4.0 Å, a range where LEED patterns suggest that the films are well ordered,[13] and that the local atomic geometry at surface steps can be reasonably assumed to be compatible with the idealized model shown in Fig. 1.

III. RESULTS AND DISCUSSION

Figure 2 displays hysteresis loops measured using the longitudinal magneto-optic Kerr effect from 2.5- and 4.0-ML-thick Fe films on W(100) at different vicinal angles. Little or no O or C signals (1% ML) were detected in AES spectra taken after film growth, suggesting that the vicinal-angle dependent switching fields (Fig. 3) exhibited by the films prior to oxygen doses are characteristic of the uniaxial step-induced anisotropy of clean Fe films. Vicinal angles were determined to an angular accuracy exceeding ±0.5° from calibration marks on the curved surface crystal, using a long focal length microscope,[3] and the switching fields H_s, for the displayed data set (which in general does not exhibit particularly sharp switching thresholds or good signal to noise) can be determined to an accuracy of about ±25 Oe. It is clear that H_s varies monotonically from small negative values for $\alpha \sim 0°$ to about 600 Oe (2.0 and 2.5 ML) and 200 Oe (4.0 ML) for $\alpha \sim 14°$. This behavior is typical for vicinal-angle-dependent switching fields associated with surface-step-induced ultrathin film magnetic anisotropy of Fe on stepped W(100).[2,3,5–7]

Figure 3 presents the vicinal angle dependence of switching fields for 2.0-, 2.5-, and 4.0-ML-thick Fe films and for selected values of oxygen coverage of the 2.5 and 4.0 ML films. The Fe film thicknesses were checked and oxygen coverages were determined by measuring the ratios of W (182
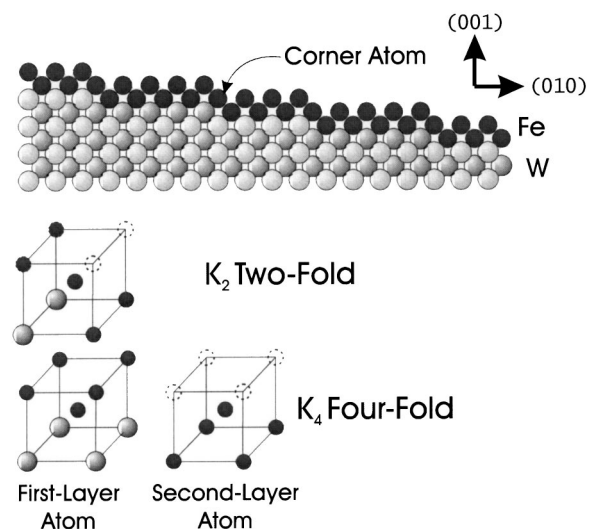

FIG. 1. Atom model of vicinal surface shows vicinal angle that yields $N = 4$ and $N = 5$ terraces. Corner atom resides at site with two-fold symmetry that produces Néel model anisotropy energy.

eV), Fe (705 eV), and O (510 eV) AES peak ratios taking into account the sensitivity factors for the AES lines.[10] No attempt was made to determine vicinal-angle-dependent oxygen coverage at a given oxygen dose, but dramatic variations were not observed. Our discussion of the experimental results are confined to the most obvious general trends in the switching field dependencies illustrated in Fig. 3: (1) the clean film switching field strength increases monotonically with vicinal angle; (2) thicker films exhibit a more prominent off-set of the switching field at low vicinalities; and (3) chemisorbed oxygen significantly reduces the switching field at high vicinalities, but does not affect the magnetization. These trends were also observed in films of other thicknesses (2.8 and 3.0 ML) in the same range and with similar oxygen concentrations.

The quadratic variation of H_s vs α for low coverage (2 ML) Fe on vicinal W(100) has been observed[2,3] and can be understood within the Néel model.[3] The Néel model predicts an inverse thickness scaling of H_s at a given α, which has yet to be observed. We do not address specifically the scaling issue in the present discussion, but point out two features of our results that have bearing on the thickness scaling: at high values of α ($\alpha \sim 9°$, for example), where both 2 and 4 ML films manifest $H_s(\alpha) \gg H_c(0)$, both curves exhibit (approximately) quadratic behavior. At lower values of α, thickness dependencies in H_c complicate the analysis, and for $\alpha > 12°$ we observe the power law become invalid for 2 ML films.[2] Failure to observe inverse thickness scaling does not necessarily imply that the Néel model is invalid at low coverage.

We conclude our discussion by suggesting that the oxygen coverage dependence of H_s presented in Fig. 3 is consistent with a localized (at steps) origin of the magnetic anisotropy energy. Definitive experiments that explore oxygen adsorption on $p(1 \times 1)$Fe on vicinal W(100) are not available, but general trends in oxygen chemisorption at d-band metal surfaces[11,12] suggest that step decoration mechanisms dominate the process. Assuming the Néel (step-atom) anisot-

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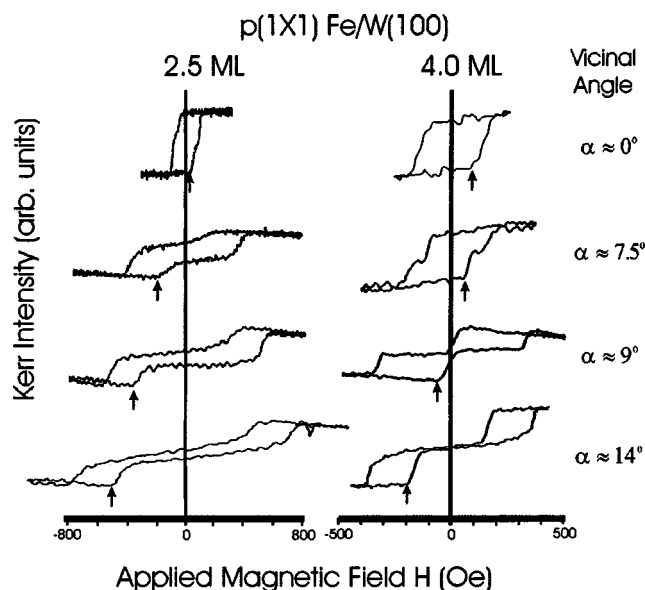H. C. Mireles and J. L. Erskine 7141

FIG. 2. Typical hysteresis loops for Fe films on vicinal W(100) showing variation of surface-step-induced switching field vs thickness and oxygen coverage. Arrows indicate M_S values.
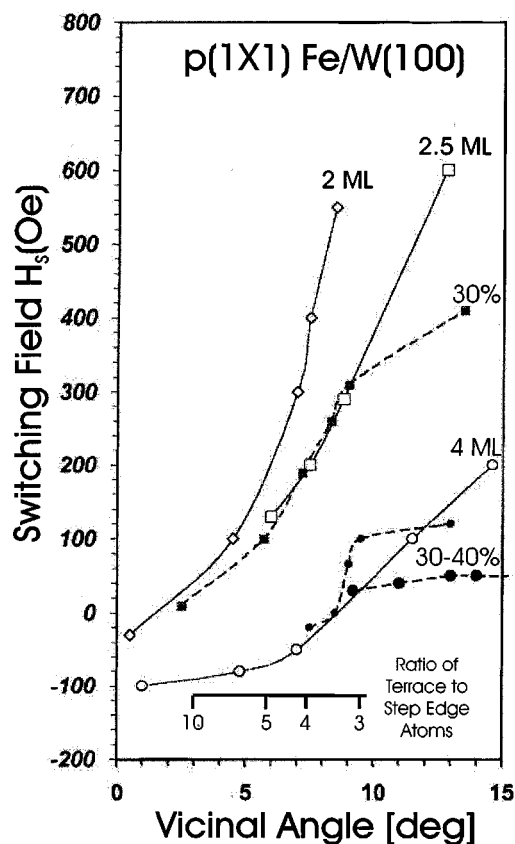

FIG. 3. Plots of switching field vs vicinality for Fe on W(100) for several film thicknesses and surface oxygen concentrations. Open points correspond to clean films; solid points correspond to films with chemisorbed oxygen ($\sim$30%). Inset shows ratio of terrace to step edge atoms at specific α.

ropy model is correct, essentially any model of chemisorption will yield a greater sensitivity of H_s to oxygen contamination at larger vicinal angles. At large vicinal angles, there are more anisotropy-producing Fe atoms per unit area that will be affected by a prescribed oxygen coverage. Realistic models[11] that include O_2 dissociation, sequential population of physisorbed and chemisorbed precursor states, and surface diffusion generally lead to step decoration at highly vicinal surfaces, and defect decoration on "flat" surfaces resulting from enhanced reactivity at low symmetry sites. Step and defect decoration effects in chemisorption can account for not only the higher sensitivity of H_s to oxygen adsorption at larger vicinal angles, but also the absence of the effects at small vicinal angles where oxygen atoms are trapped at defect sites that do not contribute to the step-induced anisotropy.

IV. SUMMARY AND CONCLUSIONS

Surface-step-induced magnetic anisotropy of $p(1\times1)$Fe films 1–4 ML thick on a graded-step-density surface was studied as a function of vicinal angle and oxygen coverage. The switching field versus vicinal angle for clean surfaces increases monotonically, and can be fit reasonably well to a power-law function $H_s \alpha \alpha^2$ up to $\alpha=10°$ for thin (2 ML) films. The power-law behavior also applies reasonably well to clean 4-ML-thick films after allowing for the $H_c=0$ behavior at small vicinal angles. The switching field does not appear to obey an inverse thickness scaling law. Chemisorbed oxygen (at 30%–40% ML) does not significantly affect the saturation magnetization M_S or the vicinal-angle dependence of H_s at small angles ($\alpha<6°$) but strongly reduces the switching fields at larger vicinal angles (while leaving M_S unaffected). This effect is consistent with step decoration

(saturating the step sites at $\sim$30% ML coverage) and with a highly localized origin of surface-step-induced anisotropy as predicted by the Néel mechanism.

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