Effect of atomic steps on the magnetic anisotropy in vicinal Co/Cu(001)

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The step-induced uniaxial magnetic anisotropy of fcc Co films grown on a curved Cu(001) substrate was investigated in the vicinal angle range of 0° to 6°. The anisotropy strength was found to depend linearly on the step density, indicating that biaxial strain due to in-plane lattice misfit is not the origin of the step-induced anisotropy. By performing Cu adsorption experiments, we found that the magnetization easy axis switches by 90° when the Co steps are decorated with ~1 atomic row of Cu per step, independent of the step density. [S0163-1829(98)51434-8]

It has been shown that uniaxial magnetic anisotropies could be generated by lattice symmetry breaking, either by the presence of a surface/interface¹ or by a uniaxial strain due to lattice mismatch.² To better understand the role of lattice symmetry breaking in the magnetic anisotropy, several groups have investigated and observed the step-induced in-plane uniaxial magnetic anisotropy in several systems.^{3,4} Moreover, investigations on Fe/stepped Ag(001) (Ref. 5) and Fe/stepped W(001) (Ref. 6) revealed that the step-induced anisotropy depends quadratically on the step density in these two systems. The step-induced magnetic anisotropy is believed to originate from two different effects: the missing bonds at the step edges and the strain within the film. Although the Néel pair-bonding model based on the missing bonds could explain the quadratic relation in bcc films,⁵ it cannot explain the observed volume-type behavior in the anisotropy.^{6–8} Currently, only the biaxial strain due to the in-plane lattice misfit has been considered for the volumetype anisotropy,^{7,9} but the strain near the step edge should be more complicated than the biaxial strain due to the lattice misfit in the normal direction. In addition, the biaxial strain also gives a quadratic relation between the step-induced anisotropy and the step density, making it difficult to separate the pair-bonding effect and the biaxial strain effect in a bcc film. To understand how these two effects contribute to the step-induced magnetic anisotropy, it becomes very important to investigate fcc films as a function of step density because the pair-bonding effect and the biaxial strain effect produce a different step-density dependence of the anisotropy, making it possible to isolate the role of each mechanism. In this paper, we present a systematic investigation of the relation between the step-induced magnetic anisotropy and the step density in a stepped fcc film. We report that the step-induced anisotropy in fcc Co/stepped Cu(001) depends *linearly* on the step density, which shows that the anisotropy does not originate from the biaxial strain. To further explore the nature of the step-induced anisotropy, we also performed Cu adsorption experiments on the stepped fcc Co film as a function of step density.

A 10 mm diameter Cu(001) single crystal was polished into a curved shape with the step edges parallel to the [110] direction. The curved substrate provides a continuous range for the vicinal angle (α) from 0° to 6°. The crystal was first mechanically polished down to 0.25 μ m diamond paste, followed by an electropolish.¹⁰ The substrate was cleaned *in situ* by cycles of Ar⁺ sputtering at 2–5 keV and annealing at 600–700 °C. Unless otherwise noted, the Co films were epitaxially grown onto the Cu substrate at room temperature with a growth pressure less than 1×10^{-9} torr. The magnetic properties of the films were measured *in situ* by the surface magneto-optic Kerr effect (SMOKE) using a He-Ne laser (632.8 nm; beam diameter 0.2 mm). For all films studied, no polar loops were observed so that the Co magnetization was always in the film plane. For measurement on the stepped surfaces, the reflection angle of the SMOKE laser beam was used to determine the local vicinal angle. A slit was placed in the path of the reflected beam to improve the vicinal angular resolution to better than 0.25°.

To investigate the step-induced magnetic anisotropy, an 8-monolayer (ML) Co film was deposited onto the substrate. Figure 1 shows representative SMOKE hysteresis loops with the applied magnetic field perpendicular to the step edges. The split loops with zero magnetic remanence show that the magnetization easy axis of the Co film is parallel to the step edges, consistent with the results in the literature.^{3,7,8} The shift field (H_S) of the split loops is argued to be proportional



FIG. 1. Hysteresis loops for an 8-ML Co film on stepped Cu(001) substrate at different vicinal angles (α). The magnetic field is applied perpendicular to the step edges. The shift field (H_S) measures the strength of the step-induced uniaxial anisotropy.

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FIG. 2. The shift field (H_S) in Fig. 1 as a function of the vicinal angle (α) . The solid line is a linear fit of H_S vs α .

to the strength of the step-induced uniaxial magnetic anisotropy.¹¹ Figure 2 displays the measured results of H_s at different vicinal angles (α). The data can be well fit with a linear relation between H_s and α . Thus, we conclude that the step-induced uniaxial anisotropy depends *linearly* on the step density in this system.

One important consequence of this result is that the stepinduced anisotropy in Co/stepped Cu(001) does not originate from the volume-type biaxial strain. The biaxial strain will produce a uniaxial anisotropy of the form $K_v u_{\zeta}^2$, where ζ =[001]. Rotating to the film coordinates and considering in-plane magnetization⁵ lead to a volume-type in-plane uniaxial anisotropy: $K_v \alpha^2 u_y^2$ (i.e., quadratic relation), where y is in the film plane and perpendicular to the step edges. Since the experimentally observed relation is linear, the biaxial strain cannot make a significant contribution to the step-induced anisotropy.

The linear dependence can be explained by the nearest neighbor Néel pair-bonding model. For a stepped fcc (001) film with step edges parallel to $[1\overline{10}]$, the missing bonds at the step-edge atoms lead to the step-induced anisotropy per unit volume of

$$E_a = -\frac{K}{2daL} \left(2u_{\eta}^2 + 3u_{\zeta}^2 + 2\sqrt{2}u_{\eta}u_{\zeta} \right).$$
(1)

Here **u** is the unit vector of the magnetization, *a* is the atomic layer spacing (1.8 Å), d is the film thickness, L is the terrace length (tan $\alpha = a/L$), $\zeta = [001]$, and $\xi = [110]$ and $\eta = [110]$ are parallel and perpendicular to the step edges, respectively. Additionally, the inclusion of the biaxial strain only modifies the coefficients of Eq. (1) but not the functional form,⁹ so this functional form can be viewed as a purely pair-bonding effect. A rotational coordinate transformation from the crystal $\xi \eta \zeta$ frame to the film xyz frame,⁵ where the z axis is normal to the film plane, and the x and y axes (in the film plane) are parallel and perpendicular to the step edges, respectively, leads to a leading term of $-K\alpha u_v^2/da^2$ for inplane magnetization $(u_z=0)$, therefore giving an α -linear dependence of the step-induced anisotropy. The same calculation for bcc leads to a quadratic dependence.⁵ Thus, we see that the α dependence is well predicted in the Néel model by considering only the missing bonds at the step edge. This model, however, does not give a complete picture of the step-induced anisotropy because experiments show that the



FIG. 3. Hysteresis loops of 8-ML Co grown on $\alpha = 5.4^{\circ}$ stepped Cu(001) before and after the growth of 0.09 ML of Cu. (a) Without Cu adsorption. (b) Cu adsorption at room temperature. (c) Cu adsorption at $T \approx 90$ K. (d) After warming sample (c) to room temperature for 1 h.

anisotropy does not have a 1/d thickness dependence,^{6–8} indicating that strain effects inside the Co film should also be important.

To understand the strain effect on the interior Co atoms, it is useful to realize that the Néel pair-bonding model is also applicable to interior atoms where the nearest-neighbor bonds are not missing but modified by the strain. There are 12 nearest-neighbor bonds for each interior Co atom: 8 along $[\pm 1,0,\pm 1]$ and $[0,\pm 1,\pm 1]$ ("diagonal" bonds) forming a body-centered-tetragonal cell with $c/a = \sqrt{2}$, and 4 along $[\pm 1, \pm 1, 0]$ ("horizontal" bonds) being approximately in the film plane. For the diagonal bonds, we find that the strain effect produces the same anisotropy functional form as for the bcc case (c/a=1), except for an additional u_{ℓ}^2 term which should give an α^2 dependence of the anisotropy in a stepped film. For the horizontal bonds, however, the leading term due to the strain will be the u_n^2 term which should give an α -linear dependence of the anisotropy in a stepped film. This probably explains why the volume-type strain leads to an α -linear dependence in the fcc film but not in the bcc film where no horizontal nearest-neighbor bonds are present.

To further understand the relation between the stepinduced anisotropy and the local environment at the step edges, we performed Cu adsorption experiments on the stepped Co film. It was shown that a minute amount of Cu adsorbates on the stepped Co film at room temperature switches the magnetization easy axis by 90° (Ref. 12) and that most of the adsorbed Cu atoms at room temperature tend to attach to the Co steps.¹³ Thus, it has been speculated that a full row of Cu adsorbates per step is needed to switch magnetization easy axis.¹² To test this idea quantitatively, we performed Cu adsorption experiments as a function of the step density.

Before performing the α -dependent study, it is important to investigate how the location of the Cu adsorbates on the stepped Co surface affects the uniaxial anisotropy. To separate the step-edge effect and the surface effect, we compared two different samples—one with the Cu adsorbates deposited R5926



FIG. 4. (a) The normalized shift field (H_S) in Fig. 1 as a function of the Cu overlayer thickness (d_{Cu}) at two different vicinal angles. d^* is the thickness where H_S goes to zero, signaling the 90° switching of the magnetization easy axis. The solid lines are guides to the eye. (b) d^* as a function of vicinal angle (α) . The solid line is a linear fit.

at room temperature, and one with the Cu adsorbates deposited at low temperature (to reduce the Cu surface diffusion). Figure 3 shows the results of the comparison after 0.09 ML Cu was deposited onto an 8-ML stepped Co film at α $=5.4^{\circ}$. The hysteresis loop before the Cu deposition is also shown for reference [Fig. 3(a)]. After the Cu deposition at room temperature, the step-induced magnetic anisotropy is clearly suppressed [Fig. 3(b)], consistent with previous studies.¹² However, the Cu adsorption at low temperature (~90 K) results in only a slight decrease in H_{S} [Fig. 3(c)]. The Cu adsorbates at low temperature have low mobility so that they should be evenly distributed over the Co surface and the step edges. Therefore, the two adsorption experiments indicate that the reduction in H_S is mainly caused by the Cu adsorbates located at the step edges. To verify this idea, the low-temperature adsorbed film was warmed up to room temperature to allow the Cu adsorbates to migrate to the Co step edges. As expected, the hysteresis loop after warming up shows a significant decrease in H_S [Fig. 3(d)]. The above experiments demonstrate that the step-induced magnetic anisotropy is localized to the step edges.

Next, we studied the magnetization switching by Cu adsorbates at different step densities. A Cu wedge was deposited on top of an 8-ML stepped Co film at room temperature, and hysteresis loops were measured along the Cu wedge to



FIG. 5. (a) Schematic drawing of the side-growth geometry. (b) The normalized shift field (H_S) in Fig. 1 as a function of the side-growth Cu thickness (d_{Cu}) at four different vicinal angles. The solid line is a guide to the eye.

determine the decrease of H_S as a function of the Cu thickness. The Cu coverage at which the H_S goes to zero signals the 90° easy-axis switching,¹² and is denoted by d^* [Fig. 4(a)]. The jump in the $\alpha = 4.3^{\circ}$ curve between 0.04–0.05 ML of Cu is due to a substrate defect as indicated by a diffused spot in the reflection beam. Figure 4(b) shows the relation between d^* and the vicinal angle α . The linear relation between d^* and α shows that it is the amount of Cu at the step edges that determines the magnetization easy axis. A recent theoretical calculation shows that electronic hybridization between Cu and Co favors the magnetization perpendicular to the Co/Cu boundary.¹⁴ The linear slope (\sim 1.4) in Fig. 4(b) is greater than one, indicating that the amount of Cu at d^* is greater than one row per step. To minimize the artifacts caused by the terrace length fluctuations and the nonperfect mobility of the Cu at room temperature, we deposited the Cu adsorbates in a side-growth geometry shown in Fig. 5(a). Since the Cu atoms are directed toward the step edge, this growth geometry should help the Cu reach the Co step edge. In addition, each Co step will receive the same amount of Cu (independent of step density), and realizes a full row of Cu decoration when the deposition time corresponds to an equivalent 1 ML of Cu in the normal growth geometry. Figure 5(b) shows the normalized H_s as a function of the sidegrowth Cu thickness at four different α . The four curves roughly fall onto a single universal curve with H_S approaching zero at ~ 1 atomic row of Cu, indicating that the magnetization switching occurs when there is ~ 1 atomic row of Cu at the Co step edge, *independent* of the step density.

Microscopically, the Cu adsorbates at the step edge create four diagonal Cu-Co bonds to the Co atoms on the lower terrace and one horizontal Cu-Co bond to the Co atoms on the upper step edge. The Néel pair-bonding model suggests that it is the modification of the horizontal bonds that contribute most to the anisotropy change in the Cu adsorption experiments. Two consequences come naturally from this analysis. First, additional Cu decoration after the first row of Cu should only weakly modify the anisotropy since they will

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only modify the diagonal bonds. Evidence of this behavior¹² seems to confirm our analysis. Second, the effect of the Cu adsorbates should be independent of the step density because both the step-induced anisotropy and the anisotropy modification by the Cu decoration come from horizontal bonds.

In conclusion, we observed a linear dependence of the step-induced magnetic anisotropy on the step density in the Co/stepped Cu(001) system. The Cu adsorption experiments performed at low temperature and room temperature indicate that the magnetization easy-axis switching is caused only by

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the Cu adsorbates located near the step edges. With normal and side growths of the Cu adsorbate, we found that the switching occurs when there is about one atomic row of Cu per step, independent of the step density. The Néel pairbonding model suggests that modifications to the horizontal bonds rather than to the diagonal bonds are responsible for the above observations.

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