Unicrystal Co-alloy media on Si(110)

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Unicrystal Co–alloy/Cr/Ag films, which exhibit a single, in-plane easy axis orientation, were epitaxially grown on hydrofluoric acid etched Si(110) single crystal substrates by sputter deposition for the purpose of the systematic study of Co–alloy magnetocrystalline anisotropy. The orientation relationship was studied by x-ray $\theta/2\theta$ diffraction, pole figure ϕ scan, and transmission electron microscopy, and it was determined to be Co(1010)[0001]||Cr(112)[110]||Ag(110)[001]||Si(110) [001]. The ϕ scan also showed two twin-related orientations of Cr grains. The easy axis hysteresis loops had a square shape, while the hard axis loops showed zero openness. The uniaxial anisotropy constants K_1 and K_2 of the unicrystal Co and CoCrTa films were determined from torque and hard axis hysteresis loop measurements. © 1999 American Institute of Physics. [S0021-8979(99)60908-2]

Magnetocrystalline anisotropy is an important property of Co alloys. While the anisotropy field determines the maximum achievable coercivity in a Co–alloy thin film,^{1,2} the anisotropy constants dictate the thermal stability of the constituent grains.³ Both of these properties are key factors in the pursuit of a higher coercivity to obtain high linear density and a smaller grain size to reduce medium noise. Hence, better control of and knowledge about anisotropy constants are essential as one attempts to envision the limits of Co alloys for future high density recording.

We have successfully developed a new epitaxy process to fabricate highly oriented Co-alloy films by the use of single crystal Si substrates. In previous work we reported the epitaxial growth of the bicrystal Co-alloy/Cr/Ag films on Si(001) wafers.⁴ In this article, we report the growth of the unicrystal Co-alloy films on epitaxial Cr/Ag templates sputter deposited on hydrofluoric acid (HF)-etched Si(110) substrates. These unicrystal Co-alloy films exhibit a single, inplane Co easy axis orientation. With the single hard and easy axes in the film plane, these films can be used to determine directly the anisotropy constants by either torque or hard axis hysteresis loop measurements. These methods are preferred to the field dependence of rotational hysteresis.⁵ While single crystal MgO(110) substrates were also used to grow unicrystal Co-alloy films,⁶ Si substrates are of interest since the wafers are readily available and inexpensive. Hence, this unicrystal epitaxial film structure provides a pathway for an extensive, systematic fundamental study of the magnetocrystalline anisotropy as functions of processing conditions, alloy composition, temperature, etc.

As shown in Fig. 1, the epitaxial orientation relationship for the unicrystal films is $Co(10\overline{1}0)[0001] \|Cr(112)$ $[1\overline{1}0] \|Ag(110)[001] \|Si(110)[001]$. It is noted that a 4×4 mesh of Ag unit cells fits very well onto a 3×3 mesh of Si unit cells, with a small mismatch of 0.4%. This is consistent with the 4-to-3 lattice match at the Ag(001)/Si(001) interface as reported in our previous work on bicrystal Co–alloy/Cr/Ag/HF-Si(001) films.⁴

The thin-film fabrication and characterization details have been described previously.⁴ The epitaxial orientation relationship was investigated with both x-ray $\theta/2\theta$ diffraction and pole figure ϕ scan. While the conventional $\theta/2\theta$ method only shows the crystal planes parallel to the film surface, the ϕ scan detects the diffraction from crystal planes that are not parallel to the film surface and thus provide information about the in-plane orientation of the grains. As an example, to obtain a {004} pole ϕ scan spectrum for a Si(110) substrate, the sample is tilted 45°, which is the angle between the (110) plane and the (100) or (010) planes. The sample is then rotated about its surface normal for 360° while the intensity of the Si{004} reflection is recorded versus the rotation angle ϕ .



FIG. 1. Orientation and interatomic spacing relationships between Si(110), Ag(110), Cr(112), and Co($10\overline{10}$) lattices.



FIG. 2. X-ray $\theta/2\theta$ diffraction spectra of: (a) a Ag(750 Å)/HF–Si(110) film, (b) a Cr(500 Å)/Ag(750 Å)/HF–Si(110) film, and (c) a Co(500 Å)/Cr(500 Å)/Ag(750 Å)/HF–Si(110) film.

The anisotropy constants K_1 and K_2 can be determined by least square fitting the torque curves $T(\theta)$ to

$$\frac{T}{V} = -\frac{\partial}{\partial \theta} [K_1 \sin^2(\theta - \lambda) + K_2 \sin^4(\theta - \lambda)]$$
$$= -(K_1 + K_2) \sin 2(\theta - \lambda) + \frac{K_2}{2} \sin 4(\theta - \lambda).$$
(1)

Here, V is the sample volume and θ is the angle between the field H and the easy axis of the unicrystal film. λ is the angle between H and the sample saturation magnetic moment m_s , and it is computed from

$$T = -m_s H \sin \lambda. \tag{2}$$

The anisotropy constants can also be determined by fitting the hard axis m(H) loops to

$$\frac{m_s H}{V} = 2K_1 \left(\frac{m}{m_s}\right) + 4K_2 \left(\frac{m}{m_s}\right)^3, \quad |m| \le m_s.$$
(3)

The $\theta/2\theta$ x-ray diffraction spectra for Ag, Cr/Ag, and Co/Cr/Ag films grown on HF-Si(110) are shown in Fig. 2. Only strong Ag(220), Cr(112), and Co(10 $\overline{10}$) diffraction peaks are observed in these spectra, which strongly implies the epitaxial nature of these films. The ϕ scan spectra of the Co/Cr/Ag/HF-Si(110) sample are shown in Fig. 3, along with cubic crystal (110), (112), and $Co(10\overline{1}0)$ stereographic projections that are necessary for the interpretation of the spectra. As can be seen, two diffraction peaks that are 180° apart are found in the Si{004} pole scan spectrum [Fig. 3(a)] of the single crystal Si(110) substrate. They correspond to the two $\{100\}$ poles in the cubic crystal (110) stereographic projection [Fig. 3(a')], which are also 180° apart along the dotted circle which shows the ϕ scan path. The two peaks corresponding to the Ag{002} poles are also 180° apart in Fig. 3(b), agreeing with the stereographic projection [Fig. 3(b')]. They appear at the same ϕ positions as the two peaks in the Si{004} pole spectrum, confirming the parallel relationship between the Si[001] and Ag[001] directions. The $Cr{110}$ pole spectrum [Fig. 3(c1)] shows two peaks that are again 180° apart, as anticipated from the projection in Fig. 3(c'). Their locations are shifted by 90° when compared to



FIG. 3. (a) Si{004} pole, (b) Ag{002} pole, (c1) Cr{110} pole, (c2) Cr{002} pole, and (d) Co{10 $\overline{11}$ } pole ϕ scan spectra of a Co(500 Å)/Cr(500 Å)/Ag(750 Å)/HF–Si(110) film. The stereographic projections are for (a'), (b') cubic crystal (001), (c') cubic crystal (112), and (d') Co(10 $\overline{10}$).

the two peaks in the Ag $\{002\}$ pole scan, indicating that the Cr $[1\overline{10}]$ direction is parallel to the Ag[001] direction.

The cubic crystal (112) stereographic projection in Fig. 3(c') only shows one (001) pole. Two diffraction peaks 180° apart, however, are observed in the Cr{002} pole scan [Fig. 3(c2)], indicating an extra pole as denoted by the × and (001)' in Fig. 3(c'). This suggests that there exist two twinrelated orientations of Cr grains in the Cr(112) film. They may emerge from the Cr/Ag epitaxial interface or result from Cr growth twinning. In bcc metals, the (112) plane is the most common twinning plane, and the twinning direction is $[11\overline{1}]$.⁷ The resulting two orientations of Cr grains have (112) planes parallel to the substrate plane, and the atomic configurations are mirror images about the $(11\overline{1})$ plane.



FIG. 4. (a) Si[110] zone axis electron diffraction pattern of a Ag(750 Å)/ HF–Si(110) film, and (b) simulated Si[110] zone axis electron diffraction pattern of Ag(110)[001] $\|$ Si(110)[001] bilayer.



FIG. 5. (a) Ag[110] zone axis electron diffraction pattern of a Co(500 Å)/Cr(500 Å)/Ag(750 Å) film grown on HF–Si(110), and (b) simulated Ag[110] zone axis electron diffraction pattern of Co(1010)[0001]]|Cr(112)[110]||Ag(110)[001] trilayer (not all double diffraction spots are included).

Finally, good agreement is also found between the Co{1011} pole scan [Fig. 3(d)] and the Co(1010) projection [Fig. 3(d')]. An orientation relationship of Co[0001] Cr[110] is also determined from the observation that two peaks in the Co spectrum appear at the same positions as those in the Cr{110} pole spectrum. The small peak width indicates a fairly good single orientation of the Co grain *c* axes.

The orientation relationship is further confirmed in the electron diffraction patterns shown in Figs. 4 and 5, both of which agree well with the simulated patterns. The complex yet regular distribution of the low intensity double diffraction spots in Fig. 4(a) is due to the 4-to-3 Ag/Si lattice match. The well defined Co(0002) spot in Fig. 5(a) also indicates good c axis alignment.

The torque curve of the Co/Cr/Ag/HF–Si(110) sample shown in Fig. 6(a) is a skewed sinusoid with a period of 180°. The anisotropy constants determined from the curve are $K_1 = 1.55 \times 10^6$ erg/cm³ and $K_2 = 1.30 \times 10^6$ erg/cm³. This K_1 is much smaller than the value reported for a bulk Co single crystal ($K_1 = 4.1 \times 10^6$ erg/cm³ and $K_2 = 1.0$ $\times 10^6$ erg/cm³).⁸ Given the good alignment of the Co grain



FIG. 6. (a) Torque curve, (b) easy axis and (c) hard axis loops of a Co(500 Å)/Cr(500 Å)/Ag(750 Å)/HF–Si(110) film.



FIG. 7. Easy and hard axis loops of a CoCrTa(500 Å)/Cr(500 Å)/Ag(750 Å)/HF–Si(110) film.

easy axes, the small K_1 cannot be explained by an easy axis orientation dispersion decreasing the torque curve amplitude. It is conjectured that Co stacking faults may develop during the sputter deposition and be responsible for this decrease. This will be the subject of a further study.

A square hysteresis loop with a coercivity of about 200 Oe is observed along the easy axis [Fig. 6(b)], indicating a coercivity mechanism dominated by wall motion. The inplane hard axis loop shows a curve with virtually zero openness, with a remanence squareness S < 0.02 [Fig. 6(c)]. This also confirms the almost perfect easy axis alignment. The anisotropy constants determined from the hard axis loop agree very well with those obtained from the torque curve. As can be seen, the hard axis loop falls almost exactly on the open circles which are the points calculated using the anisotropy constants determined from the torque curve. The hard axis loop is not a straight line; rather it shows an apparent curvature as a result of a non-negligible K_2 .

A unicrystal Co₈₄Cr₁₃Ta₃/Cr/Ag/HF–Si(110) film was also prepared. A substrate bias of -170 V was applied during the deposition of the CoCrTa layer. The anisotropy constants are determined to be $K_1=2.10\times10^6$ erg/cm³ and K_2 $=0.12\times10^6$ erg/cm³. The almost straight hard axis loop shows an anisotropy field of 7.6 kOe (Fig. 7), and indicates a negligible K_2 .

In summary, we have successfully fabricated unicrystal Co-alloy thin-film media on Cr(112)/Ag(110)/HF-Si(110) by sputter deposition. The epitaxial orientation relationship was determined, and the uniaxial anisotropy constants of unicrystal Co and CoCrTa films have been determined.

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