

Epitaxial Ag templates on Si(001) for bicrystal CoCrTa media

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Ag thin films were sputter deposited on hydrofluoric acid-etched Si(001) single crystal substrates and employed as templates for the epitaxial growth of Cr(001) films and consequently bicrystal CoCrTa(11 $\bar{2}$ 0) films. The orientation relationship was determined to be bicrystal CoCrTa on Cr(001)[100]||Ag(001)[110]||Si(001)[110]. X-ray diffraction analysis showed only strong Ag(002) peaks throughout the Ag film thickness range of 50–1500 Å. Atomic force microscopy showed that almost continuous Ag films can be achieved in the thickness range of 500–1000 Å, which result in the highest coercivities in CoCrTa films whose magnetic properties were found to vary with the Ag template thickness and surface morphology. The periodic in-plane angular variation of magnetic properties and torque curves with a four-fold symmetry were confirmed in the bicrystal CoCrTa films. © 1997 American Institute of Physics. [S0021-8979(97)28908-5]

A Co-alloy thin-film medium with a bicrystal microstructure, in which a Co(11 $\bar{2}$ 0) thin film with two orientation variants is grown epitaxially on Cr(001) single crystal,¹ provides a new system for the study of magnetocrystalline anisotropy.² In bicrystal Co/Cr films, the easy axes (i.e., *c* axes, or [0001] directions) of two crystallographically orthogonal variants of Co grains lie along either the Cr[110] or Cr[1 $\bar{1}$ 0] directions. If the volume fractions of the two variants are equal, a four-fold symmetry is expected in the in-plane angular dependence of the magnetic properties and torque curves.² Two effective easy axes emerge along the Cr[100] and Cr[010] directions yielding higher values of coercivity (H_c), remanence squareness (S), and coercivity squareness (S^*), while the Cr[110] and Cr[1 $\bar{1}$ 0] directions become effective hard axes with lower H_c , S , and S^* . Several articles have reported successfully fabricated bicrystal thin-film samples on NaCl(001),³ Cr(001),² MgO(001),⁴ and LiF(001)⁵ single crystal substrates. In this study, we report the use of Ag thin films epitaxially grown on hydrofluoric acid (HF)-etched Si(001) wafers as templates for the growth of bicrystal CoCrTa/Cr thin films. Si substrates are of interest since the wafers are readily available and inexpensive, and the fabrication process presented in this article is fairly simple. Hence, this bicrystal system opens possibilities of both extensive fundamental materials studies and the use of inexpensive oriented substrates for nonrotating storage media.

An HF-etched Si single crystal substrate, with the SiO₂ layer stripped away, presents a hydrogen-terminated surface without reconstruction.⁶ The hydrogen covalently bonds to the Si surface, terminating the otherwise dangling Si bonds, and acts to passivate against contamination of the substrates when exposed to ambient air. Ag was reported to grow on the Si(001) surface with a cube-on-cube orientation relationship, i.e., Ag(001)[110]||Si(001)[110].⁷ The misfit between the lattice constants of Ag(fcc, $a=4.09$ Å) and Si (diamond cubic, $a=5.43$ Å) is -24.7% (very close to $1/4$), yet it is noted that geometrically a 4×4 mesh of Ag unit cells fits

very well onto a 3×3 mesh of Si unit cells, with a mismatch of only 0.4%. A comparison of the crystallographic structures and lattice constants of Ag, Cr(bcc, $a=2.88$ Å), and Co₈₄Cr₁₃Ta₃(hcp, $a=2.54$ Å, $c=4.16$ Å)⁸ leads to an anticipated epitaxial relationship of bicrystal CoCrTa on Cr(001)[100]||Ag(001)[110], as shown in Fig. 1. The lattice mismatch at each of these interfaces can be calculated from the interatomic spacings shown: Cr to Ag= -0.2% , Co₈₄Cr₁₃Ta₃ to Cr= 7.8% (perpendicular to the Co *c* axis) and 2.0% (along the Co *c* axis). With such an orientation relationship, Si[110] and Si[1 $\bar{1}$ 0] become the directions of the effective easy axes, and Si[100] and Si[010] the effective hard axes.

Ag, Cr, and Co₈₄Cr₁₃Ta₃ thin films were deposited sequentially by rf diode sputtering in a Leybold–Heraeus Z-400 sputtering system. The base pressure was about 5×10^{-7} Torr. The Ar sputtering gas pressure was fixed at 10 mTorr and the sputtering power density was about 2.3

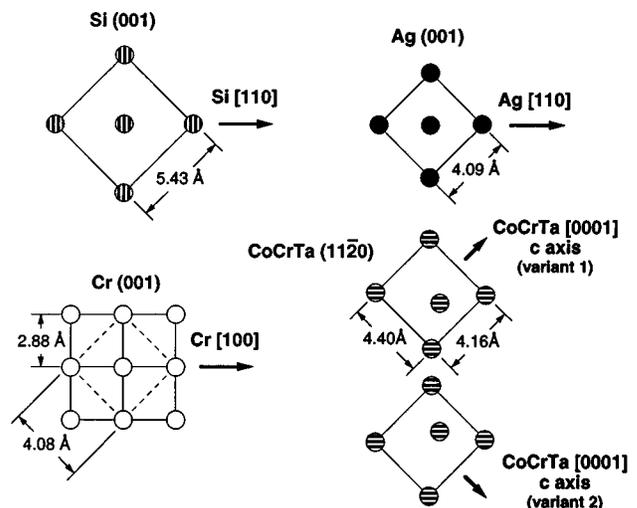


FIG. 1. Orientation and interatomic spacing relationships between Si(001), Ag(001), Cr(001), and bicrystal CoCrTa(11 $\bar{2}$ 0) lattices.

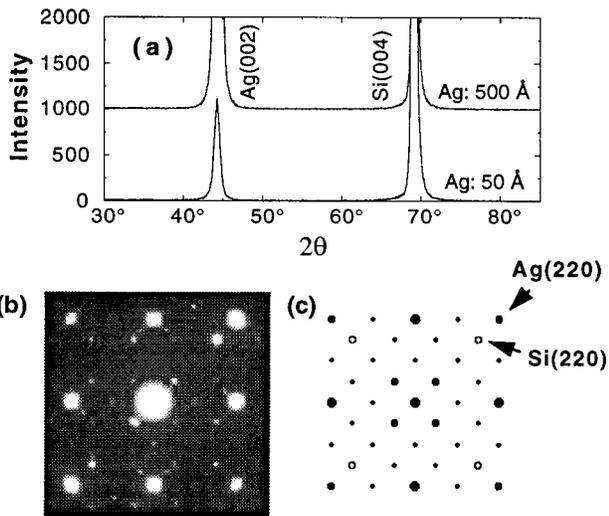


FIG. 2. (a) XRD spectra of two Ag/HF-Si films, (b) Si[001] zone axis electron diffraction pattern of a Ag(500 Å)/HF-Si film, and (c) simulated Si[001] zone axis electron diffraction pattern of Ag(001)[110]||Si(001)[110] bilayer.

W/cm². A substrate bias of -170 V^8 was applied during the deposition of CoCrTa films, while no bias was applied during the Ag or Cr deposition. The microstructure of the films were investigated by a Rigaku x-ray diffractometer with a Cu

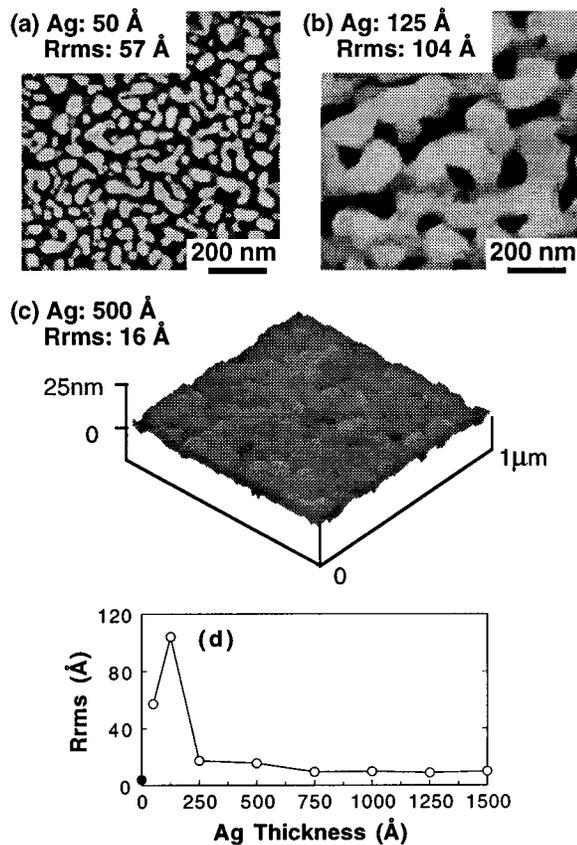


FIG. 3. AFM images of the surfaces of the Ag/HF-Si films with the Ag thickness at (a) 50 Å, (b) 125 Å, (c) 500 Å, and (d) a plot of Ag surface roughness vs Ag film thickness, in which the solid circle at the thickness of 0 Å refers to the bare HF-Si surface.

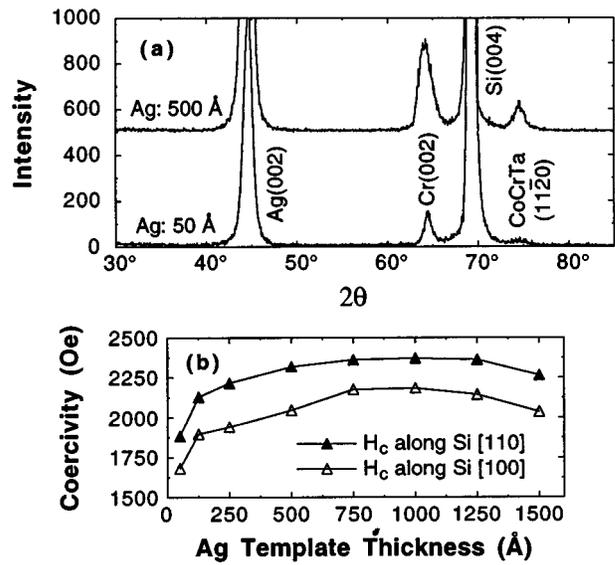


FIG. 4. (a) XRD spectra of two CoCrTa/Cr/Ag/HF-Si films, and (b) coercivity dependence on the Ag template thickness along Si[110] and Si[100] directions of the CoCrTa/Cr films. CoCrTa and Cr thicknesses are fixed at 200 and 300 Å, respectively.

$K\alpha$ radiation and a Philips EM420T transmission electron microscope. The surfaces of the Ag films were examined with a Dimension 3000 atomic force microscope (AFM). The magnetic measurements were performed on a Digital Measurement Systems vibrating sample/torque magnetometer.

The x-ray diffraction (XRD) spectra for two representative Ag/HF-Si(001) samples are shown in Fig. 2(a). Only strong (002) diffraction peaks are observed for the Ag films. The epitaxy implied in the XRD spectra is confirmed in the Si[001] zone axis electron diffraction pattern [Fig. 2(b)], which agrees well with the simulated pattern shown in Fig. 2(c). The complex yet regular distribution of the low intensity double diffraction spots in Fig. 2(b) is due to the 1/4 misfit between the Ag and Si lattice constants and is characteristic of the overlapping bilayer structure with a fixed orientation relationship. X-ray diffraction also shows that, throughout the thickness range of 50–1500 Å being studied, Ag films only exhibit strong (002) peaks, leading to the belief that a good epitaxy with the HF-Si(001) is established in very thin films and continues as the films grow thicker.

The growth of Ag on Si(001) was proposed to be in the Stranski–Krastanov, or the layer-plus-island mode: after the initial formation of one or several 2D monolayers, the 3D growth of islands begins.⁷ Or, Ag islands may nucleate at specific sites on an imperfect Si surface, then grow in size with material deposited until they touch each other. As revealed in Fig. 3(a), the surface topograph of a 50 Å Ag film clearly displays an island structure. As the film thickness increases, the neighboring islands begin to coalesce with each other to form a weblike network at 125 Å, as seen in Fig. 3(b). When the Ag film thickness is increased to 250 Å, however, a more continuouslike film forms. Further increasing the thickness results in almost continuous Ag surfaces which maintain a similar morphology to that of a 500 Å film

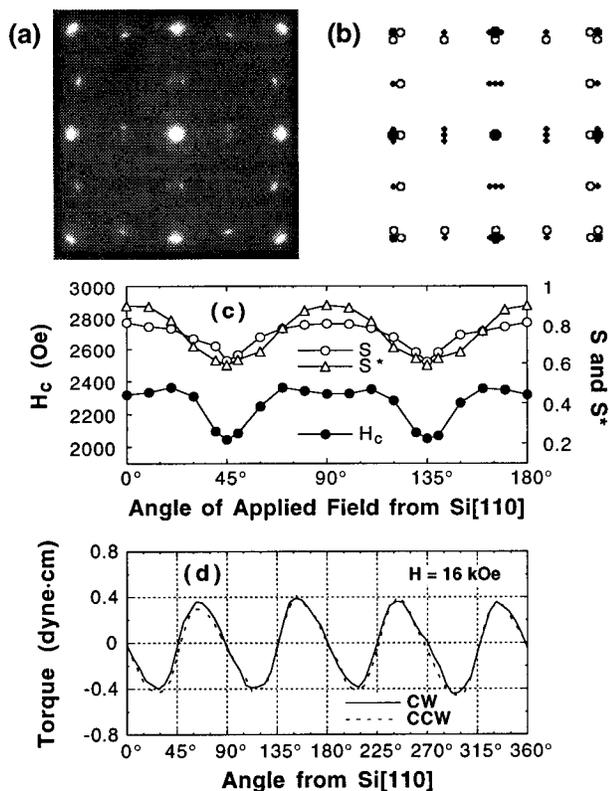


FIG. 5. (a) Cr[001] zone axis electron diffraction pattern of a CoCrTa/Cr film grown on a 500 Å Ag template, and (b) simulated Co[112̄0]/Cr[001] zone axis electron diffraction pattern of bicrystal Co/Cr bilayer. (c) In-plane angular variation of the magnetic properties, and (d) in-plane torque curve of a CoCrTa(200 Å)/Cr(300 Å)/Ag(500 Å)/HF-Si film.

[Fig. 3(c)] except for a steady expansion in the surface feature size. The evolution of the Ag surface morphology is also reflected in Fig. 3(d), the plot of the surface root-mean-square roughness (R_{rms}) vs the film thickness (a bare HF-etched Si surface has a R_{rms} of about 4 Å). For the 50 Å Ag film, a R_{rms} of 57 Å is found to be higher than the nominal film thickness. The surface roughness rises to 104 Å and yet becomes smaller than the film thickness on the 125 Å Ag film. When the film thickness is increased to 250 Å, the roughness decreases dramatically ($R_{\text{rms}}=17$ Å), and then it stays nearly constant for almost continuous surfaces as the Ag film thickness is further increased.

For the same thicknesses of CoCrTa/Cr thin films grown on these Ag templates of different thicknesses, XRD spectra show larger Cr(002), and accordingly larger CoCrTa(112̄0) peak intensities for the Ag template thickness at 500–1000 Å and lower intensities on very thin Ag films [Fig. 4(a)]. The coercivity is small for the CoCrTa/Cr films grown on very thin Ag templates, but rises to an almost constant typical value of 2300 Oe (along Si[110]) when the Ag template

thickness is greater than 500 Å, and drops again as the template thickness goes beyond 1250 Å [Fig. 4(b)]. Although a good Ag/HF-Si(001) epitaxy is achieved even for Ag films as thin as 50 Å, it appears that the higher coercivity is obtained from the CoCrTa films when the Ag template is sufficiently thick for its surface to become continuous. The surface roughness for a 125 Å thick Ag template is larger than that on a 50 Å Ag film (the ratio of the R_{rms} to the film thickness, however, is smaller), but the connected weblike surface structure seems to enhance the epitaxial growth and the coercivity of a CoCrTa(200 Å)/Cr(300 Å) film when compared to the island structure. The decrease in coercivity on very thick Ag templates is also accompanied by significantly expanded Ag surface features. The growth of the Cr films on the Ag templates with different surface morphology at different thickness may play a role in the magnetic properties of CoCrTa films and will be the subject of further studies.

Figure 5(a) shows the Cr[001] zone axis electron diffraction pattern of a CoCrTa/Cr film, which agrees well with the simulated pattern in Fig. 5(b). The periodic variation of the magnetic properties as plotted in Fig. 5(c) is further evidence of the bicrystal nature of CoCrTa films.^{2,9} Also confirmed is the parallel relationship between the Cr[100] and Si[110] directions. Furthermore, the periodicity of 90° in the in-plane torque curve [Fig. 5(b)] not only indicates a bicrystal structure, but also that the volume fractions of two CoCrTa orientation variants are almost equal.²

In summary, we have successfully fabricated bicrystal CoCrTa/Cr thin-film media on Ag templates sputter deposited on HF-etched Si(001) wafers. The epitaxial orientation relationship was determined, and the surface morphology of the Ag films and the resulting magnetic properties of the CoCrTa films have been studied. The optimal thickness of the Ag template to maximize coercivity for our current process has been determined to be 500–1000 Å.

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