Structural Analysis of Multilayered Co/Noble Metal Films with Extended 3-step Model Profile Fitting

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We have studied the annealing effect on structural changes of multilayered Co/Au, Co/Pd, and Co/Pt films, using the extended 3-step model profile fitting. This model takes account of two types of fluctuations, which are included in a periodic thickness and in a mixed layer between Co and noble metals. The profile fitting is a comparison between XRD experimental peaks and theoretical calculation peaks. As a result, for Co/Au films, the mixed layers decreased after 1.5h-annealing, and the interfaces became sharper since Co and Au is a eutectic system. On the other hand, for Co/Pd films, the mixed layers increased after 12h-annealing since Co and Pd is an isomorphous system. For Co/Pt films, the lattice strain was taken into consideration so as to succeed the profile fittings. As a result, the mixed layers of Co/Pt films increased after 12-annealing, and the lattice strain was reduced with annealing.

Keywords: multilayered Co/noble metal film, multilayered structure, extended 3-step model, X-ray diffraction, lattice strain

1. INTRODUCTION

Multilayered Co/noble metal films exhibit a large perpendicular magnetic anisotropy. They have been studied for high-density recording media such as magneto-optical disks and hard disks. The perpendicular magnetic anisotropy of these films are based on an interface between Co layers and noble metal layers. Therefore, it is very important to analyze their interface structure. In this paper, we report the structural changes of multilayered Co/Au, Co/Pd, and Co/Pt films with annealing, using the extended 3-step model profile fitting. These profile fittings with the extended 3-step model that take account of two types of fluctuations are a useful method to analyze the interface structure in detail. Furthermore, we studied the lattice strain of Co/Pt films, which prevented the usual profile fitting.

2. EXPERIMENTAL

Multilayered Co/Au, Co/Pd, and Co/Pt films were fabricated onto the rotating glass substrates with dual-source RF magnetron sputtering method, using Ar as a sputtering gas. Table I shows the sample structures. These samples were annealed in vacuum (1×10^{-4} Pa) at 300℃ for Co/Au films, at 400℃ for Co/Pd and Co/Pt films, keeping 0.5-48h respectively. XRD was measured under 40kV, 200mA with Cu-Kα_1 radiation, scanning 1.3-15 deg in the low angle region and 30-50 deg in the high angle region. Structural changes of all samples were analyzed with a profile fitting method. In the low angle region, the optical thin film model based on the dynamical theory was made use of theoretical calculations. [1] In the high angle region, we assumed the extended 3-step model based on the kinematical theory.

Table I Structure of samples

Sample	Structure
Co/Au	$[14.0/53.0\,Å]^{30}$
	2010 Å
Co/Pd	$[14.0/44.0\,Å]^{30}$
	1740 Å
Co/Pt	$[14.0/44.0\,Å]^{30}$
	1730 Å

RESULTS and DISCUSSION

3.1 Extended 3-step model

Structural analysis with profile fitting method is a comparison between XRD experimental peaks and theoretical calculation peaks. First of all, for profile fittings, periodic thickness of multilayered Co/noble metal films must be determined in the low angle region, using the optical thin film model based on the dynamical theory. Structural analysis with profile fittings for the interfaces between Co and noble metals is performed in the high angle region by the extended 3-step model based on the kinematical theory, using the periodic thickness determined in the low angle region. Schematic view of multilayered Co/noble metal films for the extended 3-step model is shown in Fig.1.

Fig.1 shows stacking atoms in the periodic thickness Λ which is stacked by N times in total. The lattice spacing and the atomic planes of each atom are expressed d_x and n_x. (x=a, b, and c) Generally, it is very difficult to fabricate multilayered films that have an ideal periodic structure. Therefore, we have to take into consideration two types of fluctuations. The first fluctuation $\Delta\Lambda$ was assumed in the periodic thickness, and the second fluctuation δd was assumed in the mixed layers.

The intensity of XRD peaks I (Q) is given by

$$I(Q) = L(Q)|F(Q)|^2 \qquad (1)$$

Here L(Q) is Laue function , and F(Q) is the layer structure factor. The periodic thickness Λ fluctuates around at the average value $\Lambda' = (n_a d_a + n_b d_b)$ with a Gaussian distribution function $\exp[-(\Lambda - \Lambda')/\sigma^2]$. Thus, Laue function is given by

$$L(Q) = \frac{1 + \exp(-N\sigma^2Q^2/2) - 2\exp(-N\sigma^2Q^2/4)\cos(N\Lambda'Q)}{1 + \exp(-\sigma^2Q^2/2) - 2\exp(-\sigma^2Q^2/4)\cos(\Lambda'Q)} \qquad (2)$$

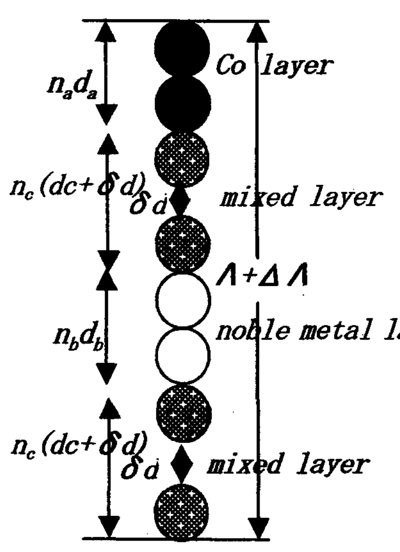

Fig.1 Schematic view of extended 3-step model

Assuming that the lattice spacing d_r fluctuates around at the average value d_c with a Gaussian distribution function $\exp[-(d_r - d_c)^2/\sigma_m^2]$, the layer structure factor F(Q) is given by

$$|F(Q)|^2 = f_a^2(Q)L_a(Q) + f_b^2(Q)L_b^2(Q)$$

$$+4f_c^2(Q)\frac{1+\exp[-n_c\sigma^2Q^2] - 2\exp[-n_c\sigma^2Q^2/2]\cos(n_c d_c Q)}{1+\exp[-\sigma^2Q^2] - 2\exp[-\sigma^2Q^2/2]\cos(d_c Q)}$$

$$\times\cos^2(\lambda_b Q/2)\exp(-\sigma^2Q^2/4)$$

$$+2f_a(Q)f_b(Q)L_a^{1/2}(Q)L_b^{1/2}(Q)\cos(\Lambda Q/2)$$

$$+\frac{2f_a(Q)f_c(Q)L_a^{1/2}}{1+\exp[-\sigma^2Q^2] - 2\exp[\sigma^2Q^2/2]\cos(d_c Q)}\cos(\lambda_b Q/2)\exp(-8\sigma^2Q^2)$$

$$\times\{\exp[-(n_c+1)\sigma^2Q^2/2]\cos[(n_c-1)d_c Q/2]$$

$$-\exp[-n_c\sigma^2Q^2/2]\cos[\Lambda Q/2+(n_c+1)d_c Q/2]$$

$$-\exp[-n_c\sigma^2Q^2/2]\cos[(n_c+1)d_c Q/2]$$

$$+\cos[\Lambda Q/2-(n_c-1)d_c Q/2]\}$$

$$+\frac{2f_b(Q)f_c(Q)L_b^{1/2}}{1+\exp[-\sigma^2Q^2] - 2\exp[\sigma^2Q^2/2]\cos(d_c Q)}\cos(\lambda_b/Q)\exp(-\sigma^2Q^2/8)$$

$$\times\{\exp[-(n_c+1)\sigma^2Q^2/2]\cos[\Lambda Q/2+(n_c+1)d_c Q/2]$$

$$+\cos[(n_c-1)d_c Q/2]\}$$

$$-\exp[\sigma^2Q^2/2]\cos[\Lambda Q/2-(n_c+1)d_c Q/2]$$

$$-\exp[-\sigma^2Q^2/2]\cos[(n_c+1)d_c Q/2] \qquad (3)$$

3.2 Structural analysis with profile fittings

3.2.1 Low angle profile fittings

The profile fitting in the low angle region was performed to determine the periodic thickness. Fig.2 shows the low angle profile fitting for Co/Au films. The periodic thickness of Co/Au films was 27 atomic planes. Similarly, the periodic thickness of Co/Pd and Co/Pt films was 27 and 26 atomic planes respectively.

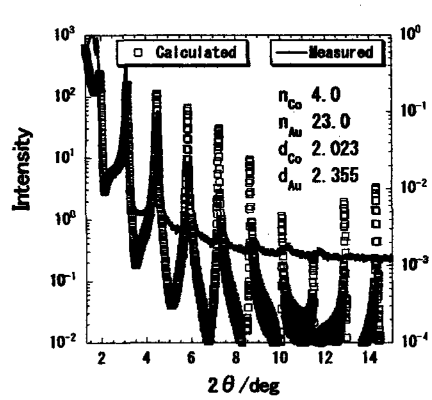

Fig. 2 Low angle profile fitting for Co/Au films

3.2.2 High angle profile fittings

The profile fitting in the high angle region was performed to analyze the changes of interfaces in detail. Fig.3 shows the extended 3-step model profile fittings. As a result of profile fittings, the mixed layers decreased from 2 to 0 atomic planes in Co/Au films, while they increased from 2 to 5 atomic planes in Co/Pd films. For Co/Pt films, the profile fittings could not be done similarly in the high angle region. It seemed that Co/Pt films had a lattice strain.

3.2.3 Lattice spacing of multilayered Co/Pt films

Fig.4 shows the annealing effect on (111) lattice spacing of Pt films. The lattice spacing of Pt (111) is quoted from JCPDS. (2.265 Å) [2] On the other hand the lattice spacing of Pt films was 2.292 Å as-sputtered. These results are considered that Pt films have lattice strain at the stacking process.

However, the lattice strain of Pt films could be reduced with annealing, and the lattice spacing became 2.285 Å after 12h-annealing. When the annealing was continued until 48h, the lattice spacing became close to the quoted value.

Accordingly, for Co/Pt films, the profile fitting was performed on the condition that Pt layers have lattice strain. Fig.5 shows the extended 3-step model profile fittings of Co/Pt films. Fig.5-(c) shows the profile fitting for Co/Pt films before annealing, which made use of the lattice spacing 2.291 Å. Fig.5-(c)' shows the profile fitting of 12h-annealing, which made use of lattice spacing 2.285 Å. As a result of these profile fittings, the mixed layers of Co/Pt films decreased from 0 to 1 atomic layers with annealing since Co and Pt is an isomorphous system. Here, Fig.6 shows the profile fitting in the low angle region for Co/Pt films, using the lattice spacing 2.291 Å.

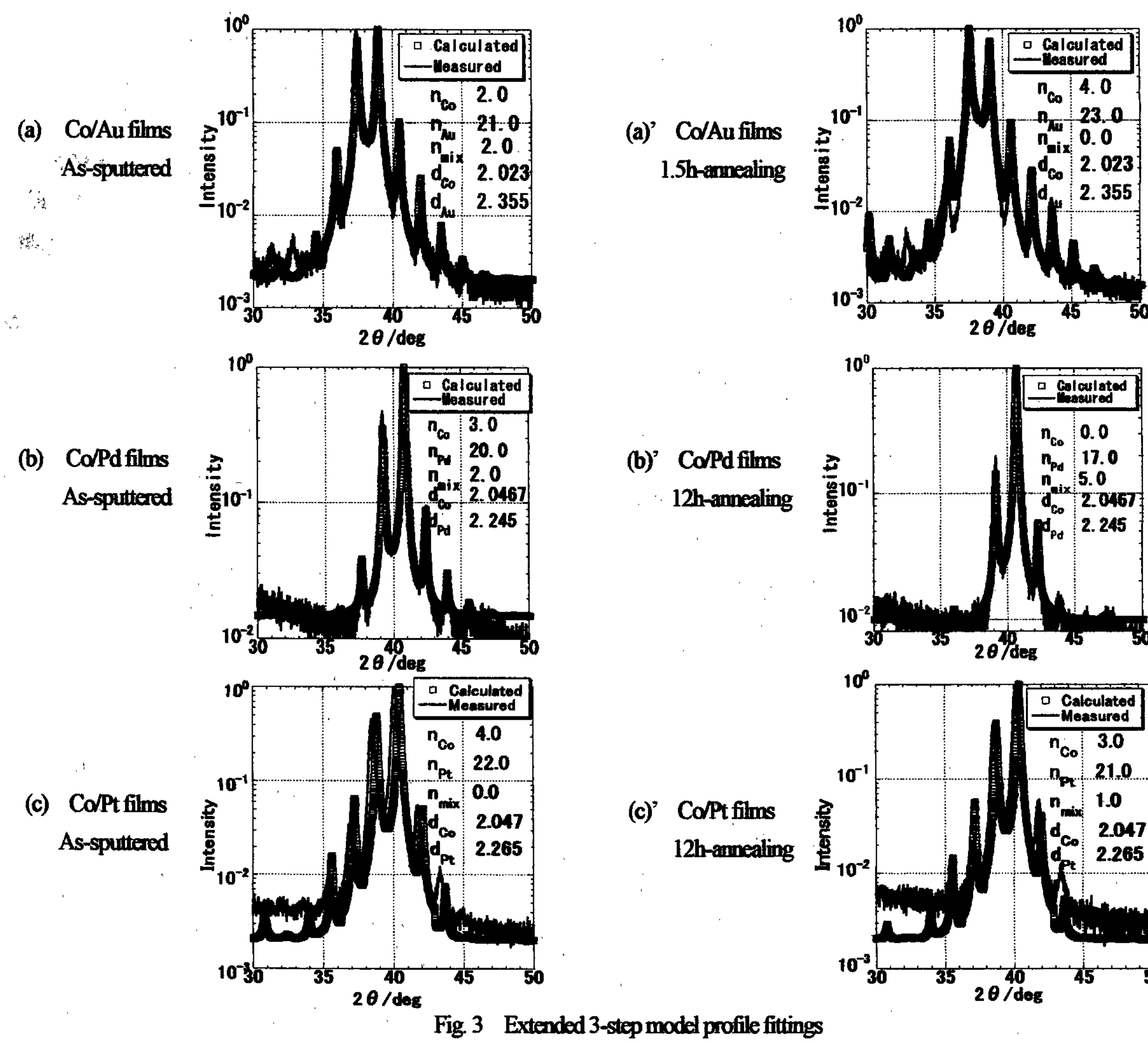

Fig. 3 Extended 3-step model profile fittings
(a) Co/Au films, (b) Co/Pd films, and (c) Co/Pt films

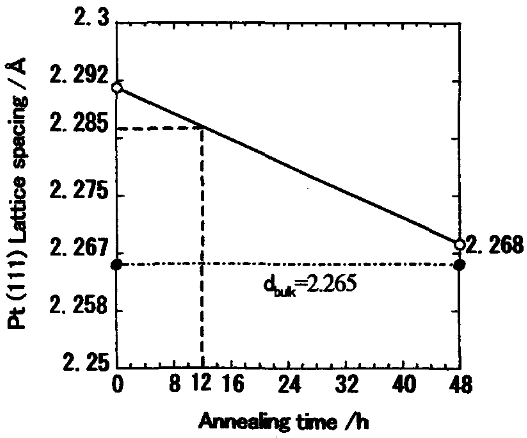

Fig.4 Change of (111) lattice spacing for Pt sputtering films with annealing

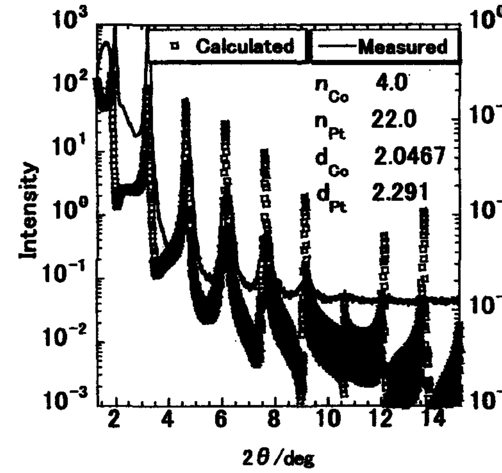

Fig.6 Low angle profile fitting for Co/Pt films (as-sputtered)

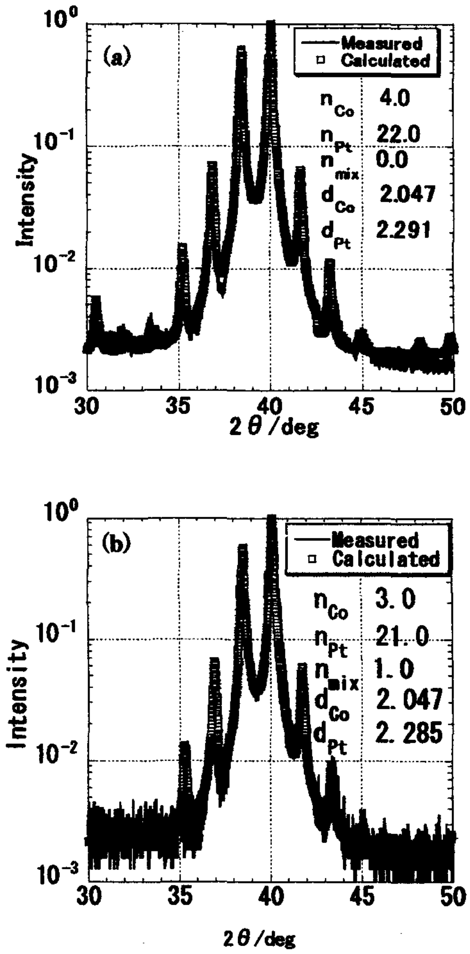

Fig.5 High angle profile fittings for Co/Pt films (a) as-sputtered, (b) 12h-annealing

It is obvious that the profile fitting, using d_{Pt}=2.291 Å, could be done successfully similar to the profile fitting in the high angle region.

4.CONCLUSION

We performed the structural analysis for multilayered Co/Au, Co/Pd, and Co/Pt films from a comparison of XRD experimental peaks and theoretical calculation peaks with the extended 3-step model. For Co/Pt films, Pt was considered to have lattice strain during the stacking process. Therefore, the lattice strain of Pt was taken into consideration. As a result of profile fitting, for Co/Au films, the mixed layers decreased, and the interfaces became sharper with annealing since Au and Co is a eutectic system. On the other hand, the mixed layers of Co/Pd and Co/Pt films increased with annealing, since Pd and Co is an isomorphous system.

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