Structural Analysis of Co/Pd, Co/Au, and Co/Pt Multilayered Films with Extended 3-step Model Profile Fitting

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We have studied the annealing effect on structural changes of Co/Pd, Co/Au, and Co/Pt multilayered 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 X-ray diffraction (XRD) experimental peaks and theoretical calculation peaks. As a result of the profile fitting, for Co/Pd films, the mixed layers increased after 12h-annealing since Co and Pd is an isomorphous system. On the other hand, 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. For Co/Pt films, the lattice strain of Pt was considered to perform the profile fitting. Not only, the mixed layers of Co/Pt films increased after 12h-annealing, but also the lattice strain was reduced.

Keywords: multilayered structure, extended 3-step model, X-ray diffraction, lattice strain.

1. INTRODUCTION

Co/Noble metal multilayered films such as Co/Pd, Co/Au, and Co/Pt films exhibit a large perpendicular magnetic anisotropy. They have been studied for next-generational high-density recording media such as magneto-optical disks (MO) and perpendicular recording hard disks. [1] Though the perpendicular magnetic anisotropy seems to be some effects of the interface between Co layers and Noble metal layers, the details has not been clear. Therefore, it is very important study to analyze interfacial structure. In this paper, we report the structural changes of Co/Au, Co/Pd, and Co/Pt multilayered films with annealing, using the extended 3-step model profile fitting. Profile fitting with extended 3-step model is very useful method for the analysis of interface and layered structure. Extended 3-step model was improved considering two kinds of fluctuations in our study. Furthermore, we studied the lattice strain of Co/Pt films that prevented a usual profile fitting.

2. EXPERIMENTAL

Co/Noble metal multilayered films were fabricated by a dual-source RF magnetron sputtering onto the rotating glass and polyimide substrates at ambient temperature. The shutter attached for the each target controlled the each layer thickness of multilayered films. Layered structure of multilayered films are as follows: $[Co/Pd]_N=[1.41nm/4.41nm]_{30}$,$[Co/Au]_N=[1.41nm/5.28nm]_{30}$,$[Co/Pt]_N=[1.41nm/4.37nm]_{30}$. These films were annealed in vacuum (1×10^{-4}Pa) at 573K for Co/Pd, Co/Pt films and at 473K for Co/Au films, keeping 0.5-48h respectively to examine changes structure with annealing time. XRD was performed by RIGAKU RINT-1500 with Cu-K α_1 (λ

=0.15405nm), 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. [2] In the low angle region, the optical thin film model based on the dynamical theory was made use of theoretical calculations. In the high angle region, we assumed the extended 3-step model based on the kinematical theory.

3. RESULTS and DISCUSSION

3.1 Extended 3-step model

A comparison between XRD experimental peaks and the theoretical calculation peaks was done with structural analysis with profile fitting method. In the low angle region, the periodic thickness is decided with profile fittings so that XRD peaks based on only a periodic thickness may appear. Optical thin film model considering the complex refractive index was used in the low angle region, because a multiple scattering influenced in each interfaces. [3] In the high angle region, structural changes of the interface can be analyzed with the profile fitting. Extended 3-step model, which based on the kinematical theory, was improved to contain two kinds of fluctuation. Fig.1 shows the schematic view of extended 3-step model. Periodic thickness Λ is composed of a, b and c atom, and assumed it stacked N number in total. The lattice spacing and the atomic planes of each atom are expressed dx and nx, when it assumed 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 of two types of fluctuations, $\Delta\Lambda$ and δ d.

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

$$I(Q) = L(Q)|F(Q)|^2 \tag{1}$$

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[4]

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

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[5][6]

$$\begin{aligned}
|F(Q)|^2 &= f_a^2(Q)L_a(Q) + f_b^2(Q)L_b^2(Q) \\
&+ 4f_c^2(Q)\frac{1+\exp\left[-n_c\sigma^2Q^2\right] - 2\exp\left[-n_c\sigma^2Q^2/2\right]\cos(n_c d_c Q)}{1+\exp\left[-\sigma^2Q^2\right] - 2\exp\left[-\sigma^2Q^2/2\right]\cos(d_c Q)} \\
&\times\cos^2(\lambda_b Q/2)\exp(-\sigma^2Q^2/4) \\
&+ 2f_a(Q)f_b(Q)L_a^{1/2}(Q)L_b^{1/2}(Q)\cos(\Lambda Q/2) \\
&+ \frac{2f_a(Q)f_c(Q)L_a^{1/2}}{1+\exp\left[-\sigma^2Q^2\right] - 2\exp\left[\sigma^2Q^2/2\right]\cos(d_c Q)}\cos(\lambda_b Q/2)\exp\left(-8\sigma^2Q^2\right) \\
&\times\{\exp\left[-(n_c+1)\sigma^2Q^2/2\right]\cos\left[(n_c-1)d_cQ/2\right] \\
&- \exp\left[-n_c\sigma^2Q^2/2\right]\cos\left[\Lambda Q/2 + (n_c+1)d_cQ/2\right] \\
&- \exp\left[-n_c\sigma^2Q^2/2\right]\cos\left[(n_c+1)d_cQ/2\right] \\
&+ \cos\left[\Lambda Q/2 - (n_c-1)d_cQ/2\right]\} \\
&+ \frac{2f_b(Q)f_c(Q)L_b^{1/2}}{1+\exp\left[-\sigma^2Q^2\right] - 2\exp\left[\sigma^2Q^2/2\right]\cos(d_c Q)}\cos(\lambda_b/Q)\exp\left(-\sigma^2Q^2/8\right) \\
&\times\{\exp\left[-(n_c+1)\sigma^2Q^2/2\right]\cos\left[\Lambda Q/2 + (n_c+1)d_cQ/2\right] \\
&+ \cos\left[(n_c-1)d_cQ/2\right]\} \\
&- \exp\left[\sigma^2Q^2/2\right]\cos\left[\Lambda Q/2 - (n_c+1)d_cQ/2\right] \\
&- \exp\left[-\sigma^2Q^2/2\right]\cos\left[(n_c+1)d_cQ/2\right]
\end{aligned} \tag{3}$$

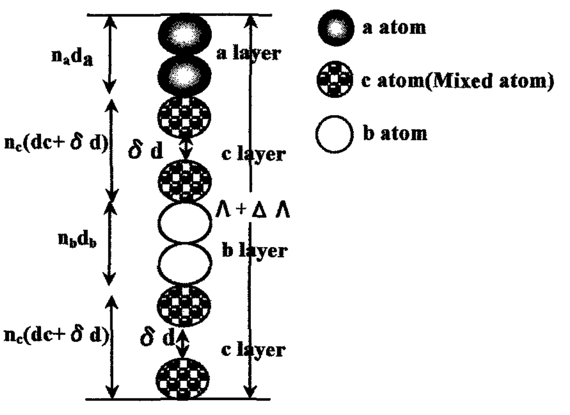

Fig.1 Schematic view of extended 3-step model

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

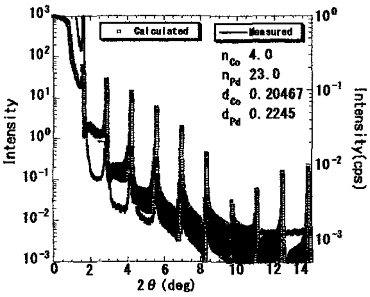

Fig.2 Low angle profile fittings for Co/Pd films

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 increased from 2 to 4 atomic planes in Co/Pd films, while they decreased from 2 to 0 atomic planes in Co/Au. Moreover, for Co/Pt films, the profile fittings could not be done in the high angle region. It seemed that Co/Pt films had a lattice strain, since only Co/Pt films fabricated on polyimide substrates were bended hard.

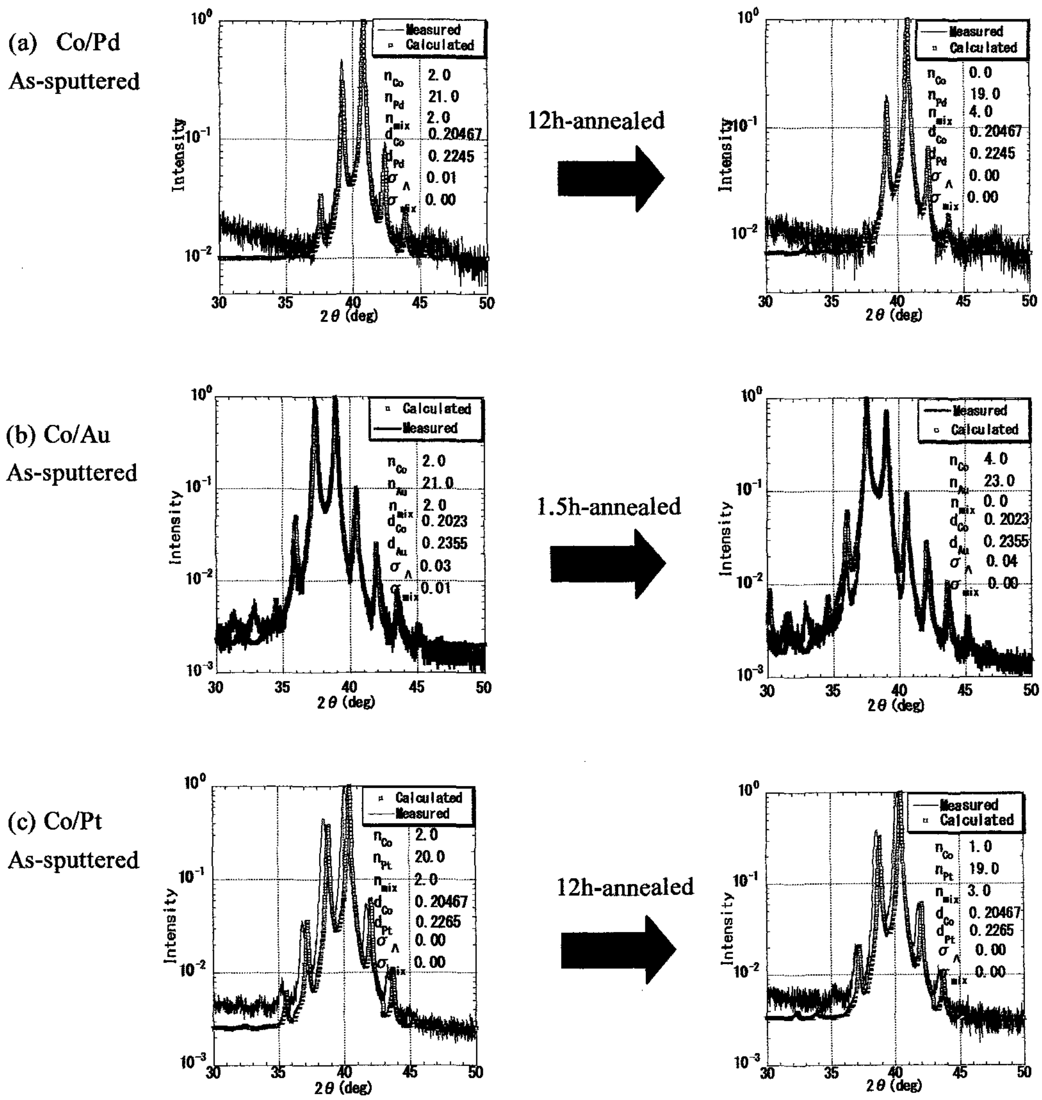

Fig. 3 Extended 3-step model profile fittings
(a) Co/Pd films, (b) Co/Au films, and (c) Co/Pt films

3.2.3 Lattice spacing of multilayered Co/Pt films

Figure 4 shows the annealing effect on (111) lattice spacing of Pt films. The lattice spacing (0.2265**nm**) of Pt (111) is quoted from JCPDS. [7] On the other hand the lattice spacing of Pt films was 0.2291**nm** 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 0.2285**nm** after 12h-annealing. When the annealing was continued until 48h, the lattice spacing became close to the bulk 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 (a) shows the profile fitting for Co/Pt films before annealing, which made use of the lattice spacing 0.2291**nm**. Fig.5 (b) shows the profile fitting of 12h-annealed, which made use of lattice spacing 0.2285**nm**. As a result of these profile fittings, the mixed layers of Co/Pt films decreased from 2 to 3 atomic layers with annealing since Co and Pt is an isomorphous system.

4.CONCLUSION

We performed the structural analysis for Co/Pd, Co/Au and Co/Pt multilayered 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. For Co/Pd films and Co/Pt films, the mixed layers of the interface increased with annealing. Since Co-Pd and Co-Pt is an isomorphous system, their alloying was promoted. On the other hand, for Co/Au films, the mixed layer decreased with annealing. Since Co-Au is a eutectic system, the separation of Co and Au relaxed the disorder of the interface, and the ideal layered structure was formed.

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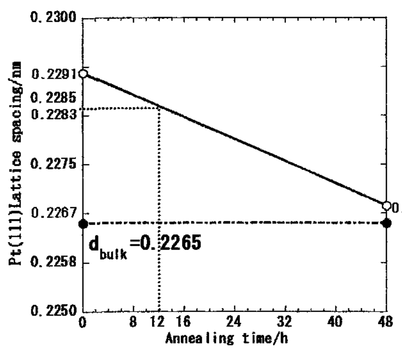

Fig.4 Change of (111) lattice spacing for Pt sputtering films with annealing

(a) Co/Pt As-sputtered

(b) Co/Pt 12h-annealed

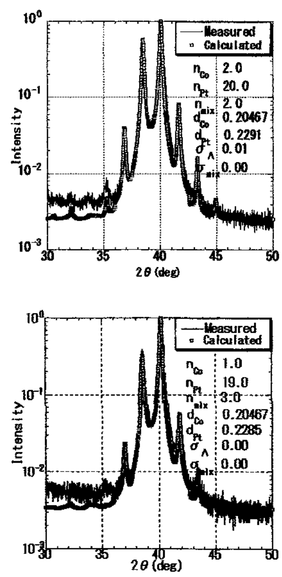

Fig.5 High angle profile fittings for Co/Pt films (a) As-sputtered, (b) 12h-annealed

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