Changes in the Composition of Sputtered Barium Ferrite Films as a Result of Scattering Due to the Collision of Sputtered Particles and Sputtering Gas

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Abstract -- In this study, we used computer simulation to investigate changes in the composition of hexagonal barium ferrite films deposited by a facing target sputtering. The iron content in the film increased as the sputtering gas pressure increased and reached a maximum value at a certain gas pressure. These changes in the film composition were explained as follows; sputtered particles scatter when they collide with sputtering gas atoms, and this scattering changes a ratio of the particles reaching the substrate. When the substrate was located to the side of the target in a facing target sputtering system, this scattering resulted in an increase in the amount of sputtered particles arriving at the substrate, although too much scattering caused the amount to decrease. Since this gas scattering depends significantly on the atomic mass of the sputtered particles, the gas pressure dependence of the amount of the iron atoms arriving differs considerably from that of the amount of barium atoms arriving. This difference leads to the changes in film composition.

I. INTRODUCTION

A hexagonal barium ferrite (BaM) thin film with an excellent magnetic properties cannot be obtained unless the film composition is controlled precisely[1]. In the sputter deposition of barium ferrite films, however, the film composition changed significantly when the deposition conditions change[2], mainly because high-energy particles bombarding the film surface caused the composition of the film to differ from that of the target material[1,2]. This high energy particle bombardment to the film surface was eliminated in facing target sputtering (FTS), which resulted in only a small change in film composition[1].

The iron content in a BaM film deposited by a FTS system, however, increases with an increase of sputtering gas pressure, reaches a maximum at a certain gas pressure, and decreases with further increases in the gas pressure. To explain these changes in the film composition with sputtering gas pressure, we carried out a computer simulation of the sputter deposition processes and found that changes in the film composition with sputtering gas pressure were mainly caused by the scattering that occurs when sputtered particles in the space between the target and substrate collide with the atoms of the sputtering gas.

In this paper, we will show the mechanisms of the composition changes caused by the scattering of sputtered particles through the collisions with sputtering gas atoms in FTS and in conventional magnetron sputtering.

II. SIMULATION OF TRANSPORT PROCESS IN SPUTTERING

A facing target sputtering system and a magnetron type sputtering system were assumed to be used for the film deposition (Fig. 1). The trajectory of each of the sputtered particles emitted from the target was calculated as shown in Fig. 2, and the amount of sputtered particles deposited on substrate was estimated. This transportation of the sputtered particles was calculated according to the model reported by Motohiro[3] and Turner[4]. The emission angles of sputtered particles from the target were assumed to be followed by cosine law. The energy distributions of iron atoms and barium atoms emitted from the target were calculated by using Thompson’s model[5]. For the iron atoms, the energy distribution emitted from pure iron target was used. For barium atoms, following parameters were used in calculating the energy distribution: atomic number, 56; atomic mass, 137.3;
atomic radius, 2.22 Å; length between atoms, 4.35 Å; bonding energy (BaO), 8.4 eV. In the simulation, 50 million atoms were emitted from the target and the amount of particles incident to the substrate was calculated at various sputtering gas pressures. It should be noted that the sputtering gas, iron, and barium differ considerably in terms of both atomic radius and atomic mass.

### III. RESULTS AND DISCUSSIONS

#### A. Facing target sputtering system

Figure 3 shows simulated examples of the amount of iron and barium atoms arriving at the substrate. The amount of atoms arriving in Fig.3 was normalized by the value obtained at 2 mTorr. It should be noted that the amount of atoms arriving increases as the sputtering gas pressure increases. This increase is explained as follows: In a facing target sputtering system, the substrate is located to the side of the target as shown in Fig.1(a). In this target-substrate arrangement, scattering of the sputtered particles by the collision with sputtering gases leads to an increase in the amount of sputtered particles arriving at the substrate. Too much scattering, however, causes the amount to decrease.

When the sputtering gas pressure increases from 2 mTorr to 5 mTorr, the amount of iron atoms arriving increases more steeply than does the amount of barium atoms arriving. On the contrary, in the gas pressure range from 5 mTorr to 15 mTorr, in contrast, the amount of barium atoms arriving increases more steeply. This difference in the gas pressure dependence is mainly due to the different atomic masses of iron and barium.

These differences in the amount of deposition particles arriving cause the film composition to change. The ratio of the amount of the iron atoms to barium atoms arriving at the substrate (arrival ratio) is equivalent to the composition of the deposited film. Figure 4 shows the changes in the ratio of the amount of iron atoms to barium atoms arriving at the substrate with sputtering gas pressure. This result indicates that the iron content in the film increases as the sputtering gas pressure increases and that it reaches a maximum at a certain gas pressure. These changes in the arrival ratio shown in Fig.4 agree qualitatively with the experimental results shown in Fig.4.

These results indicate that when other sputtering gases (such as Kr and Xe) are used in place of Ar, the gas pressure dependence of the amount of iron and barium atom arriving will differ significantly from that observed in the sputtering using argon gas. This difference will result in changes in the pressure dependence of the film composition. Figure 5 and 6 show examples of the amounts of iron and barium atoms arriving during sputtering in various gases. From these results, the changes in film composition with the changes in sputtering gas pressure shown in Fig. 7, can be derived. As the sputtering gas pressure increases from 6 mTorr, the iron content in the film deposited in Kr or Xe decreases more rapidly than does that in the film deposited in Ar. The sputtering-gas-dependent changes in film composition should thus be taken into consideration to obtain a film with the desired composition.

#### B. Magnetron sputtering system

Figure 8 and 9 show the amount of atoms arriving and the arrival ratio of iron atom to barium atom,
Fig. 5. The amount of iron atoms arriving during sputtering in Ar, Kr, and Xe.

Fig. 6. The amount of barium atoms arriving during sputtering in Ar, Kr, and Xe.

Fig. 7. Arrival ratio of iron atom to barium atom sputtered in Ar, Kr, and Xe.

respectively, sputtered in the magnetron sputtering system shown in Fig. 1(b). The substrate in the magnetron sputtering system was located in front of the target, so the amounts of both iron and barium arriving at the substrate decreased monotonically as the sputtering gas pressure increases. The amount of arrived iron atoms, however, decreased more steeply than did the amount of barium atoms. As a result, the iron content in the film decreased monotonically as the sputtering gas pressure increased. This decrease in iron content was caused by the difference between the scattering of iron atoms and the scattering of barium atoms. As the sputtering gas pressure increases, the iron atom scattering due to collisions with sputtering gas becomes more significant than the barium atom scattering.

IV. CONCLUSIONS

The transportation of sputtered particles from the target to the substrate was investigated in order to clarify the mechanisms of the composition change observed in the sputter deposition of barium ferrite films. The scattering of sputtered particles by collision with the sputtering gas was found to play an important role in changing the film composition. In addition, it should be noted that this gas scattering effect will lead to quite different gas pressure dependence of film composition when the arrangement of target and substrate in the sputtering systems is changed.

REFERENCES