Monte Carlo simulation for Magnetic Granular System with Gaussian Distribution

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1 Introduction

Magnetic granular systems have been studied for their physical interesting, i.e. spin glass properties or magnetic resistance phenomena and also for their engineering applications. Ordinary magnetic granular systems keep the homogeneous density of the magnetic granule in a non-magnetic matrix, although the each distance between nearest neighbour granules takes various values. This means magnetic granules are spread out homogeneously in non-magnetic matrix as a whole and such a granular system has no particular distribution.

But if a granular system includes localized bias, the magnetic properties will typically change comparing with homogeneous one.

Actually, on grain boundaries of Alloy 600, it is a one of Ni-base alloy, Cr depletion due to a thermal treatment forms a distribution of magnetic granules and the magnetic hysteresis curves are strongly affected by the distribution. To know the properties of magnetic granular systems with various distributions would lead a new method for controlling magnetic behavior. In this paper, magnetic hysteresis behaviors for magnetic clusters with various distributions are discussed using Monte Carlo method to reveal the mechanism microscopically.

2 Grain Boundary Magnetism of Alloy600

Ni-base superalloy Alloy600 (Inconel) has been used well as structural materials due to high mechanical strength. Originally, Alloy600 has no magnetism, but after thermal heating treatment, it becomes to show magnetic hysteresis [1,2]. Figure 1 shows experimental magnetic hysteresis curves of Alloy600 with various heating duration times at room temperature. Several experimental reports show that the magnetization occurs at Cr depletion areas around grain boundaries. Figure 2(a) is a scanning electron micrograph (SEM) around a grain boundary of Alloy600 with a duration time of 5h. Black tiny points on the boundary are carbon precipitates. Thermal heating treatment progresses to produce Cr carbide using Cr around carbons. Then Cr depletion occurs around Cr carbide on a grain boundary as shown in Fig.2(b) which is a result of Energy Dispersive X-ray Spectroscopy (EDX). The broken stoichiometry due to the Cr depletion induces magnetism and the magnetic properties depend on the distribution of Cr depletion. The distribution can be fitted as a Gaussian curve approximately as shown in enlarged view in Fig2(b).

3 Calculation Method

Monte Carlo simulation was performed to reveal the relationship between magnetic clusters with various Gaussian distribution and their magnetic properties.

A cubic system composed of 30^3 cells ($0 \leq x \leq 29$, $0 \leq y \leq 29$, $0 \leq z \leq 29$) was prepared including magnetic sites with a distribution. The distribution was decided by the fitting curve of Cr depletion degree around a grain boundary on the supposition that Cr depletion introduces magnetic moments around the depletion area. Figure 3(a) shows the Gaussian fitting curves with total number of magnetic sites N and square of standard deviation σ^2 for different duration time and Fig.3(b) shows a inside view of a model cluster including magnetic sites corresponding with N=5000 and σ^2=20 as an example.

A Hamiltonian used for the simulation includes exchange energy between nearest neighbour sites, magnetic dipole interaction and external magnetic field.

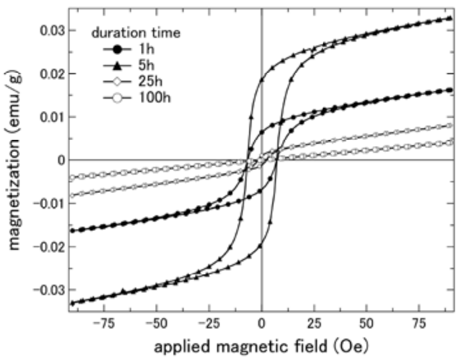

Fig. 1. Magnetic hysteresis curves for Alloy600 with various duration times.

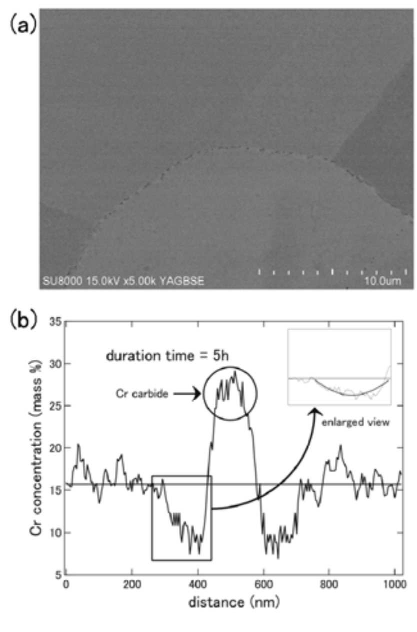

Fig. 2. (a) SEM image of grain boundary with Cr carbides and (b) Cr depletion around a grain boundary.

For more details of the Monte Carlo method for the magnetic dynamic process, see Ref. [3-5].

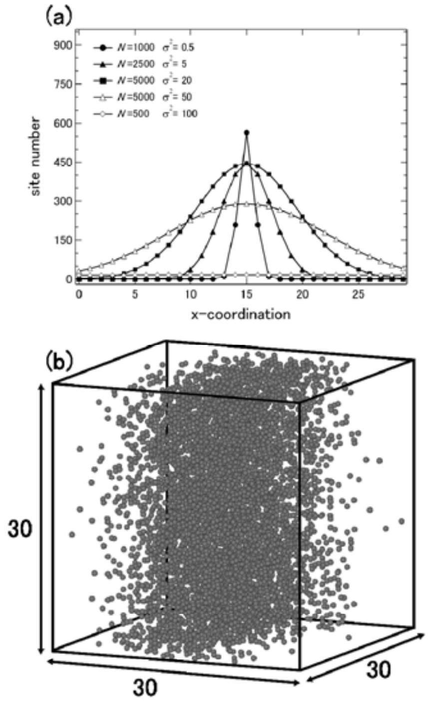

Fig. 3. (a) Various distribution of magnetic sites and (b) inside view of a cluster with N=5000 and σ^2=20.

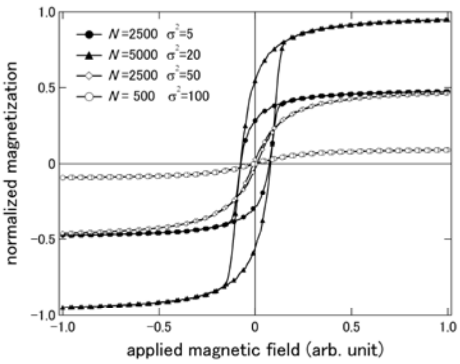

Fig. 4. Simulated magnetic hysteresis curves with various numbers of magnetic sites N and square of standard deviation σ^2.

4 Results and Discussion

Figure 4 shows calculated hysteresis curves for each distribution. It is clearly seen that magnetic properties, especially remanence M_r and coercivity H_C are strongly influenced by N and σ^2. The tendency is good correspond to experimental ones. The result means that the microscopic distribution of magnetic site controls hysteresis phenomena. Until now, many attempts to control magnetic hysteresis were performed for changing the property of whole system, e.g. new materials developments, improvement of quality of crystallization etc. Above result, however, suggests another possibility for control magnetic hysteresis by making local distribution of magnetic sites, namely, a granular with a microscopic distribution.

To grasp the relationship between the distribution and magnetic properties in wider range, the square of standard deviation σ^2 dependence of magnetic coercivity and remanece were calculated for different magnetic site number N as shown in Fig. 5. Both coercivity and remanence are increasing with decreasing of σ^2. Although the pass of magnetic property changes for concrete Alloy 600 is limited because of the unity of Cr depletion promotion process, if N and σ^2 can be selected more widely, e.g. using spin glass materials, controlling of hysteresis would be available in general.

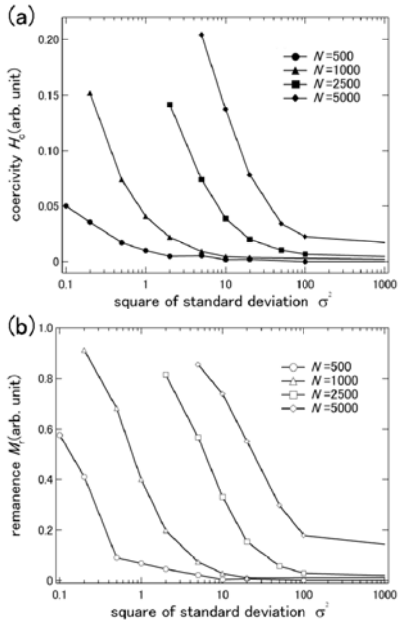

Fig. 5. Square of standard deviation σ^2 dependence of (a) magnetic coercivity H_C and (b) remanence M_r for different total magnetic site number N.

References

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