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COMPUTER SIMULATION OF MAGNETIC PROPERTIES OF SPRING MAGNETS

N. Kitajima, H. Inoue, Y. Kanai and H. Fukunaga
Department of Electrical Engineering and Computer Science, Nagasaki University,
Nagasaki, 852, Japan

Magnetic properties of model exchange-spring magnets, which are composed of magnetically soft and hard grains, were calculated by means of computer simulation. The dependence of the magnetic properties on the strength of intergrain exchange interaction and the amount of soft grains was studied. The existence of soft grains enhanced the remanence remarkably, and the remanence over $0.8M_s$ was obtained in the model magnets containing 25% or more soft grains by volume. The calculated coercivity vs. the strength of the exchange interaction curves showed a peak at a critical strength of the exchange interaction, although the remanence increased monotonously with increase in the strength of the exchange interaction. Thus the maximum energy product also reached a peak around the same critical strength. The calculated maximum energy product exceeded $300kJ/m^3$ when the magnet is assumed to be composed of Fe_3B and $Nd_2Fe_{14}B$.

I. INTRODUCTION

Recently, exchange-spring magnets, which are composed of magnetically soft and hard grains, arrested much attention because of their potential for high remanence and large maximum energy product[1]. This type of magnets has been reported in Nd – Fe – B [1,2] and Sm – Fe – N[3,4] alloy systems. In these magnets, the magnetization in soft grains is considered to be coupled to that of hard ones by the exchange interaction and is prevented from reversal even in the presence of a reversal field. Thus the exchange interaction contributes not only to the previously reported remanence enhancement but also to the coercivity enhancement in soft grains. In addition, soft grains generally have larger saturation magnetization than that of hard grains. The large saturation magnetization is also responsible for large remanence and maximum energy product of exchange-spring magnets.

As understood from the above explanation, we need to optimize the strength of the exchange coupling and the amount of the soft grains in order to obtain exchange-spring magnets with superior hard magnetic properties. Excessive strength of intergrain exchange coupling and excessive amount of soft grains would cause a drastic decrease in coercivity. As the strength of intergrain exchange coupling depends on the grain size[5], Schrefl et al. calculated M-H curves of some model exchange-spring magnets by FEM[6] varying the grain size and the amount of soft grains. However, they did not find a critical grain size at which the coercivity reaches a maximum value. Therefore simulation of magnetic properties is needed for exchange-spring magnets with wider ranges of the grain size and the amount of soft grains. In this study, we simulated magnetic properties of exchange-spring magnets by varying the strength of exchange coupling and the amount of soft grains, and found the values corresponding to the largest $(BH)_{max}$.

II. MODEL AND CALCULATION METHOD

A. MODEL MAGNET

Figure 1 shows the model magnet used in this study. The magnet consists of magnetically soft and hard cubic grains, totaling $8000(20 \times 20 \times 20)$. The magnetically hard grains have uniaxial anisotropy oriented randomly, whose anisotropy constant is K_{uH}. The soft grains were assumed to have no anisotropy($K_u = 0$) and are distributed randomly in position. The grain sizes used in our simulation assures the single domain state. The details of this assumption are discussed elsewhere[7]. The magnetization in a grain is coupled to those of six neighboring grains by the exchange interaction and to all the other grains by the magnetostatic interaction. When an external field H_a is applied in the x direction, the total energy W of the magnet is given by

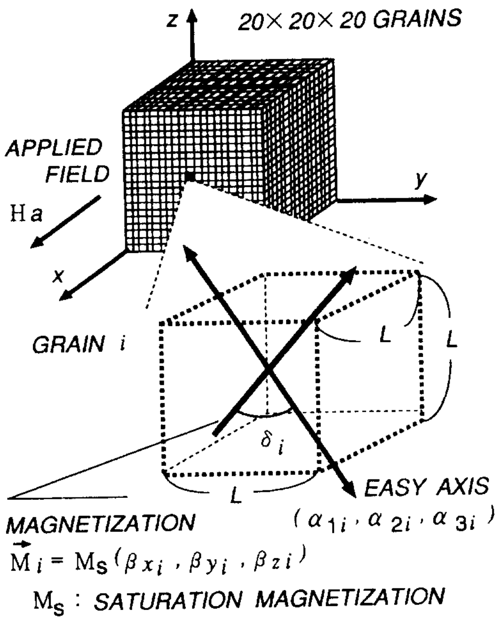

Fig.1. model magnet

$$W = \sum_{i=1}^{8000}\left\{K_{ui}V\sin^2\delta_i - \frac{J_sS}{6}\left(\sum_{j=1}^{6}\frac{\vec{M}_i}{M_s}\cdot\frac{\vec{M}_j}{M_s}\right) - \vec{M}_i\cdot\vec{H}_aV\right\} + W_m, \quad (1)$$

where S, V, K_{ui}, M_s, J_s,and W_m are the surface area and the volume of the grain, the anisotropy constant in ith grain, the saturation magnetization, the exchange interaction constant per unit surface area and the magnetostatic energy due to the local demagnetizing field, respectively. $\vec{M}_i$ and $\vec{M}_j$ are the magnetization vectors in the ith and the neighboring jth grains. Furthermore δ_i is the angle between $\vec{M}_i$ and the easy direction of the magnetization in the ith grain.

For a given $\vec{H}_a$, the functional derivatives of W with respect to β_{xi}, β_{yi} and β_{zi} satisfy

$$\frac{\delta W}{\delta\beta_{xi}} = \frac{\delta W}{\delta\beta_{yi}} = \frac{\delta W}{\delta\beta_{zi}} = 0. \quad (2)$$

Here β_{xi}, β_{yi} and β_{zi} are the direction cosines of the magnetization in the ith grain.

For example, $\delta W/\delta\beta_{xi}$ is written as

$$\frac{\delta W}{\delta\beta_{xi}} = -2K_{uH}V\left\{\alpha_{1i}\cdot(\alpha_{1i},\alpha_{2i},\alpha_{3i})\cdot(\beta_{xi},\beta_{yi},\beta_{zi}) \right.$$

$$\left. \frac{J_sS}{6K_{uH}V}\left(\sum_{j}^{6}\beta_{xj}\right) + \frac{M_s}{2K_{uH}}(H_a + H_{dxi})\right\} \quad (3)$$

where α_{1i}, α_{2i}, and α_{3i} are the direction cosines of the easy axis in the ith grain, and H_{dxi} is the x component of the demagnetizing field in the same grain.

The magnetization M of the model magnets is defined as the average of the x component of $\vec{M}_i$

B. CALCULATION METHOD

Equation (2) does not have a unique solution for a given $\vec{H}_a$. Therefore we determined the solution by rotating the magnetization in each grain so as to diminish the magneto-torque acting on the magnetization. The magnetization rotation was calculated by solving Gilbert's equation[8];

$$\left(\dot\beta_{xi},\dot\beta_{yi},\dot\beta_{zi}\right)^T = \frac{\gamma}{1+\alpha^2}$$

$$\begin{pmatrix} \alpha(\beta_{xi}^2-1) & \alpha\beta_{xi}\beta_{yi}-\beta_{zi} & \beta_{yi}+\alpha\beta_{zi}\beta_{xi} \\ \beta_{zi}+\alpha\beta_{xi}\beta_{yi} & \alpha(\beta_{yi}^2-1) & \alpha\beta_{xi}\beta_{yi}-\beta_{zi} \\ \alpha\beta_{xi}\beta_{yi}-\beta_{zi} & \beta_{xi}+\alpha\beta_{yi}\beta_{zi} & \alpha(\beta_{zi}^2-1) \end{pmatrix}\begin{pmatrix} \frac{\delta W}{\delta\beta_{xi}} \\ \frac{\delta W}{\delta\beta_{yi}} \\ \frac{\delta W}{\delta\beta_{zi}} \end{pmatrix} \quad (4)$$

where γ and α are the gyromagnetic constant and the damping parameter, respectively.

In this report, the term representing to the magnetostatic energy, W_m, was omitted because the magnetostatic interaction does not have substantial effects compared with the exchange interaction[5, 9] and its calculation consumes much time. Furthermore, the periodic boundary conditions were used in the calculation.

III. RESULTS

Figure 2 shows hysteresis loops calculated for magnets containing 25% and 50% of soft grains. In the figure, m and h are the reduced magnetization M/M_s and the reduced applies field $(M_s/2K_{uH})\cdot H_a$, respectively. When the exchange interaction parameter $\eta(=J_sS/6K_{uH}V)$ is small, the grain size is large, and the hysteresis loops are constrictive because the magnetization reversal in the soft grains is independent of the magnetization reversal in hard grains. When η is increased up to 0.118, the intergrain exchange coupling becomes larger, preventing the magnetization in soft grains from reversing.

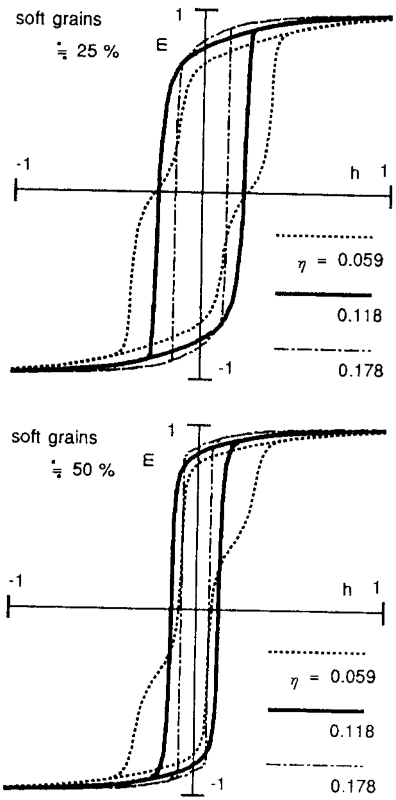

Fig.2. Reduced M-H curves.

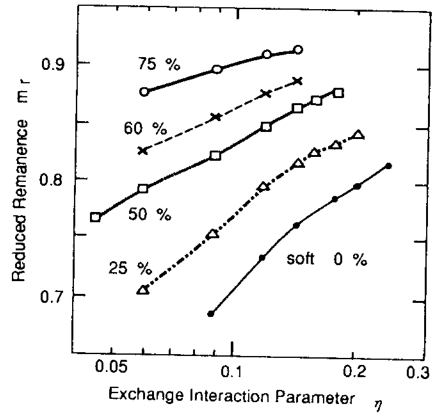

Fig.3. Reduced remanence m_r as a function of exchange interaction parameter η.

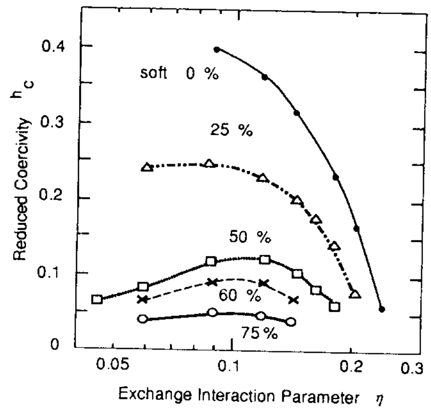

Fig.4. Reduced coercivity h_c as a function of exchange interaction parameter η.

This coupling diminishes the constrictive loops and increases the maximum energy product $(BH)_{max}$. Further increase in η (decrease in the grain size) causes clustering of grains, which decreases the reduced coercivity h_c but increases the reduced remanence m_r.

Variations of m_r and h_c are shown in Fig. 3 and 4 as a function of η. The reduced remanence m_r increases and h_c decreases with increasing η and the amount of soft grains. The increase in m_r due to an increase in soft grains can be attributed to the fact that the direction of the magnetization in soft grains is not affected by the anisotropy. The h_c vs. η curves show a peak at $\eta \simeq 0.1$, if the magnets contain more than 25% soft grains. The relationship between m_r and h_c is shown in Fig. 5. When the magnet consists of only hard grains, the locus move monotonically from the bottom-right side to the upper-left side in the figure with increasing η. In the magnets containing soft grains, the calculated curves have a critical point at which h_c reaches the maximum value. The critical points are indicated by the arrows $A_1 \sim A_4$ for the magnets containing soft grains of 25%, 50%, 60% and 75%, respectively. From the viewpoint of h_c, the value of η should be adjusted to these critical values($\eta \simeq 0.1$). Assuming the K_{uH} and M_s of $Nd_2Fe_{14}B$ alloy and $J_s = 16(\mathrm{erg/cm^2})$[5], $\eta = 0.1$ corresponds to the grain size of about 300Å. This value roughly agrees with the experimentally observed values in exchange-spring magnets[1-4]. It is also seen that m_r obtained at the critical points $A_1 \sim A_4$ increases as the amount of soft grains increases.

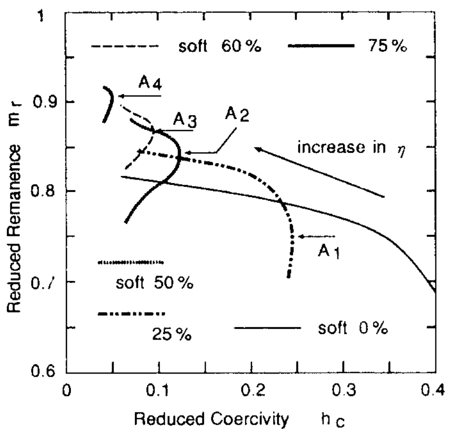

Fig.5. Relation between reduced remanence m_r and reduced coercivity h_c.

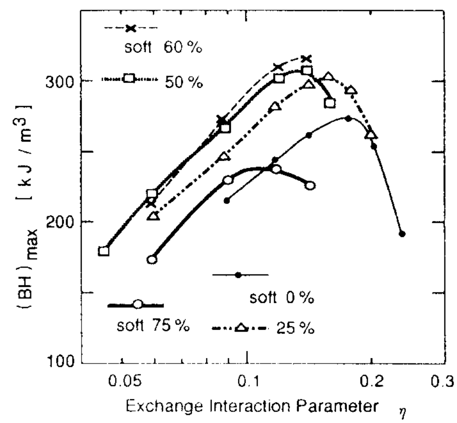

Fig.6. Maximum energy product calculated under the assumption that the magnet consists of magnetically soft Fe_3B and hard $Nd_2Fe_{14}B$ grains. The saturation magnetization of all the grains were assumed to be equal to the weighted average of those of Fe_3B and $Nd_2Fe_{14}B$.

Figure 6 shows the maximum energy product $(BH)_{max}$ calculated under the assumption that the magnet is composed of magnetically soft Fe_3B and hard $Nd_2Fe_{14}B$ grains. When η increases, $(BH)_{max}$ increases at first, reaches a maximum and then decreases drastically. If the magnets contain 25 ~ 60% soft grains, the peaks are obtained at η = 0.1 ~ 0.15. This result suggests that the increase in $(BH)_{max}$ shown in Fig. 6 is related to the increase in h_c and the disappearance of the constrictive hysteresis loops shown in Figs. 2 and 4. The calculated $(BH)_{max}$ exceeds 300kJ/m^3 for the magnets containing 25% ~ 60% Fe_3B grains.

IV. CONCLUSIONS

Magnetic properties of exchange-spring magnets were calculated by computer simulation using the micromagnetic theory. Their magnetic properties strongly depended on the strength of intergrain exchange interaction and the amount of soft grains. The existence of soft grains enhanced the remanence remarkably and the remanence over $0.8M_s$ was obtained in model magnets containing more than 25% soft grains. When the strength of intergrain exchange interaction η was varied, the coercivity vs. the strength curves had a peak. The peaks were obtained at nearly the same value of η, regardless of the amount of soft grains. When we assumed that the magnet is composed of Fe_3B and $Nd_2Fe_{14}B$, the calculated $(BH)_{max}$ exceeded 300kJ/m^3.

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