Computer Simulation of Enhancement of Coercivity in Nd-Fe-B/(Nd,Dy)-Fe-B Composite Magnets

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The coercivity \( H_c \) of Nd\(_{14}\)Fe\(_{86}\)B magnets and Nd\(_{14}\)Fe\(_{86}\)/(Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)B composite magnets were calculated by computer simulation based on the micromagnetic theory under assumptions that Nd\(_{14}\)Fe\(_{86}\)B and (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)B grains have magnetically deteriorated layers on their surfaces and diffusion of Dy from (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)B grains to Nd\(_{14}\)Fe\(_{86}\)B ones through the contacting boundaries recovers the magnetic anisotropy of the deteriorated layers of Nd\(_{14}\)Fe\(_{86}\)B grains. \( H_c \) of Nd\(_{14}\)Fe\(_{86}\)/(Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)B composite magnets increased by the diffusion of Dy from (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B grains to Nd\(_{14}\)Fe\(_{86}\)B ones and the resultant recovery of the anisotropy field of deteriorated layers of Nd\(_{14}\)Fe\(_{86}\)B grains. The \( H_c \) vs fraction of (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B grains curve were convex for the magnets with the degree of alignment between 0.94 and 0.99, which suggests that the above composite magnets have larger \( H_c \) values than the alloy-magnets with the same Dy content, and that we can save the consumption of Dy by using these composite magnets.

Keywords: (Nd,Dy)-Fe-B, coercivity, micromagnetic simulation, magnetization reversal, diffusion of Dy, magnetically deteriorated layer

1. Introduction

Recently, Nd-Fe-B sintered magnets with excellent magnetic properties were widely used for electrical devices and equipments. For such applications, a magnet is needed to have a high coercivity value even at a high temperature, typically 200°C. Although the substitution of a part of Nd for Dy is effective in increasing coercivity \( H_c \), the resource of Dy is limited and it is necessary to suppress its consumption. As one of breakthroughs for this problem, it has been reported that \( H_c \) of a small Nd-Fe-B sintered magnet is increased by the grain interface reforming due to the diffusion of a heavy rare earth element such as Dy to the grain surface of Nd\(_{14}\)Fe\(_{86}\)B [1, 2], which suggests that the importance of the surface of Nd-Fe-B grains. In this method, Dy was coated on surfaces of a magnet and was diffused to the surfaces of the grains of the magnet by annealing. Thus, the coated Dy played a role of Dy-source. The source of Dy is one of key points of this method and other sources have already reported [3, 4].

In this contribution, we assumed Nd\(_{14}\)Fe\(_{86}\)B/(Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)B composite magnets and the diffusion of Dy from (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B grains to Nd\(_{14}\)Fe\(_{86}\)B ones. Then, we varied the fraction of (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B grains, carried out a numerical simulation of magnetization reversal process in the composite magnets based on the micromagnetic theory, and clarified effects of the Dy diffusion on \( H_c \) of Nd-Fe-B/(Nd,Dy)-Fe-B composite magnets.

2. Simulation Method

2.1. Simulation Model

The atomic ratio of Dy to (Nd+Dy) in (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B grains was set at 0.3 in this study, and the model magnet consisted of 8 cubic grains (Nd\(_{14}\)Fe\(_{86}\)B and (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B ones). The number of (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B grains was varied from 0 to 8. A grain, 48 nm in size, was divided into 4096 elements as shown in Fig. 1. The direction of the easy axis of Nd\(_{14}\)Fe\(_{86}\)B and (Nd\(_{0.7}\)-Dy\(_{0.3}\))\(_{14}\)Fe\(_{86}\)B grains curve were convex for the magnets with the degree of alignment between 0.94 and 0.99, which suggests that the above composite magnets have larger \( H_c \) values than the alloy-magnets with the same Dy content, and that we can save the consumption of Dy by using these composite magnets.

Figs. 2(a) and (b) shows the variations of the anisotropy...
were determined from the previous report for single crystals [7] as indicated in Table 1. The other simulation parameters are also shown in Table 1.

Furthermore, we assumed that annealing of a composite magnet causes the diffusion of Dy from \((\text{Nd}_{0.7}\text{Dy}_{0.3})_2\text{Fe}_{14}\)B grains to \(\text{Nd}_2\text{Fe}_{14}\)B ones through the contacting grain boundaries, and that the anisotropy field of a \(\text{Nd}_2\text{Fe}_{14}\)B grain increases as indicated in Fig. 2(b), although that of a \((\text{Nd}_{0.7}\text{Dy}_{0.3})_2\text{Fe}_{14}\)B grain is kept constant.

### 2.2. Simulation method

We deduced the magnetic energy \(W\) stored in the model magnet mentioned above, considering the anisotropy, exchange, magnetostatic, and Zeeman energies. The stable direction of magnetization in each element was determined so as to minimize \(W\) for a given applied field. Details of our calculation method were reported elsewhere [8].

### 3. Simulation Results

#### 3.1. Nd\(_2\)Fe\(_{14}\)B Magnets

At first, we examined the effect of magnetically deteriorated layers on magnetic properties by varying \(R\). Fig. 3 shows typical variations of a demagnetization curve for the model magnets composed of \(\text{Nd}_2\text{Fe}_{14}\)B grains. The \(<\cos\theta>\) value was set at 1. As seen from the figure, magnetization was reversed at once except the case of \(R = 0\), and \(H_c\) increased with increasing \(R\).

For the one-dimensional model with \(<\cos\theta> = 1\), we can obtain the dependence of the nucleation field on \(R\) analytically by extending the calculation by Aharoni [9], and the nucleation field reduced by the anisotropy, \(h_n\), is given by

\[
h_n = \cos^2 \varphi + R \sin^2 \varphi, \quad (1)
\]

\[
\varphi = \frac{\sqrt{-R + h_n}}{T}, \quad (2)
\]

\[
T = D_o \sqrt{H_A M_s / 2}, \quad (3)
\]

where \(D_o\) and \(H_A\) are the thickness of the deteriorated

### Table 1 Simulation parameters.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>(\text{Nd}<em>2\text{Fe}</em>{14})B Before diffusion</th>
<th>(\text{Nd}<em>2\text{Fe}</em>{14})B After diffusion</th>
<th>((\text{Nd}<em>{0.7}\text{Dy}</em>{0.3})<em>2\text{Fe}</em>{14})B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anisotropy field</td>
<td>- Inner -</td>
<td>5.60</td>
<td>5.60</td>
</tr>
<tr>
<td>(H_A) [MA/m]</td>
<td>- Inner -</td>
<td>2.80</td>
<td>2.80</td>
</tr>
<tr>
<td>Saturation magnetization</td>
<td>- Inner -</td>
<td>1.61</td>
<td>1.61</td>
</tr>
<tr>
<td>(M_s) [T]</td>
<td>- Inner -</td>
<td>1.61</td>
<td>1.61</td>
</tr>
<tr>
<td>Grain size (L) [(\mu)m]</td>
<td>48</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exchange stiffness constant (A) [J/m]</td>
<td>(8.7 \times 10^{12})</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
layer and the anisotropy field, respectively. The solution of eqs. (1)-(3) is shown in Fig. 4, together with that of our three-dimensional calculation in this study. As seen in the figure, both results are nearly same, suggesting the reliability of our simulation. The slight deference between analytical calculation and our result would be attributed to the difference in the models because our model is three-dimensional and includes the effect of the magnetostatic interaction.

Demagnetization processes were simulated with varying \(<\cos\theta>\) and \(R\), and the obtained \(H_c\) is shown in Fig. 5 as a function of \(R\). The result for one-dimensional model was obtained by solving eqs. (1)-(3).

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reverses the anisotropy field at 50% deteriorated layers.

On the other hand, $H_c$ of the magnets with $<\cos \theta> = 1$ increased linearly with the fraction of $(\text{Nd}_{0.7}\text{Dy}_{0.3})_2\text{Fe}_{14}\text{B}$. This result is different from those for the magnets with $<\cos \theta> = 0.97$ and 0.98 shown in Fig. 6, which suggests that the magnetization reversal of perfectly aligned magnets ($<\cos \theta> = 1$) is strongly affected by unrecovered grain surfaces. In spite of the results for the magnets with $<\cos \theta> = 1$, it should be noted that the $<\cos \theta>$ values are less than 0.98 for practical magnets, and that the synthesis of composite magnets saves the Dy consumption for practical magnets.

4. Conclusions

The coercivity $H_c$ of Nd$_2$Fe$_{14}$B and Nd$_2$Fe$_{14}$B/(Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B composite magnets were calculated by computer simulation based on the micromagnetic theory under assumptions that Nd$_2$Fe$_{14}$B and (Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B grains have magnetically deteriorated layers on their surfaces, and that diffusion of Dy from (Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B grains to Nd$_2$Fe$_{14}$B ones through the contacting boundaries recovers the magnetic anisotropy of the deteriorated layers of Nd$_2$Fe$_{14}$B grains. Main results are summarized as follows.

The coercivity was improved by the recovery of the anisotropy field in magnetically deteriorated layers. Improvement in $H_c$ was significant in highly anisotropic magnets, when the anisotropy field in the deteriorated layers exceeded the half of that of the inner parts.

For Nd$_2$Fe$_{14}$B/(Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B composite magnets, it was clarified that $H_c$ increased by the diffusion of Dy from (Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B grains to Nd$_2$Fe$_{14}$B ones and the resultant recovery of the anisotropy field of deteriorated layers of Nd$_2$Fe$_{14}$B grains. The $H_c$ vs fraction of (Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B grains curve was convex for the magnets with $<\cos \theta> = 0.94-0.99$, which suggests that above composite magnets have larger $H_c$ values than the alloy-magnets with the same Dy content, and that we can save Dy consumption by using these composite magnets.

References


Fig. 6. Coercivity $H_c$ of Nd$_2$Fe$_{14}$B/(Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B composite magnets as a function of fraction of (Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B grains. We assumed diffusion of Dy from (Nd$_{0.7}$Dy$_{0.3})_2$Fe$_{14}$B grains to Nd$_2$Fe$_{14}$B ones and the resultant increase in $R$ for Nd$_2$Fe$_{14}$B grains. Details of the assumed variation of $R$ are described in the text.

