Magnetic properties of isotropic and anisotropic SmCo₅/α-Fe nanocomposite magnets with a layered structure simulated by micromagnetic theory

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(Submitted 5 November 2013; received 23 September 2013; accepted 15 October 2013; published online 13 January 2014)

Magnetic properties of anisotropic and isotropic SmCo₅/α-Fe nanocomposite magnets with a layered structure were computer-simulated with varying the stacking period, the α-Fe fraction, and temperature. The \((BH)_{\text{max}}\) values of approximately 800 and 700 kJ/m³ were achieved for anisotropic magnets at 300 and 473 K, respectively. These values roughly agree with results for SmCo₅/α-Fe with a core-shell structure, and the value at 473 K is much higher than that of Nd₂Fe₁₄B/α-Fe with a layered structure. For isotropic magnets, the largest \(H_c\) values were obtained for the stacking periods of approximately 20 and 25 nm at 300 and 473 K, respectively. The achieved \((BH)_{\text{max}}\) values were approximately 300 and 250 kJ/m³ at 300 and 473 K, respectively. The behavior of \(H_c\) was discussed in terms of the ratio of exchange energy to magnetic anisotropy one.

I. INTRODUCTION

Nanocomposite magnets are hopeful candidates for next generation magnets. Because of high Curie temperatures of Sm-Co alloys, a Sm-Co/α-Fe nanocomposite magnet is expected to possess superior magnetic properties at high temperatures. The high magnetocrystalline anisotropy of Sm-Co alloys enables the presence of a large amount of α-Fe in the magnet while necessitating a small grain size. Therefore, the microstructural design is an important issue in developing Sm-Co/α-Fe magnets. First-principle calculations have been reported on effects of microstructure on magnetic properties of Sm-Co/α-Fe powders and layered structures. We have already calculated the temperature dependence of the magnetic properties of SmCo₅/α-Fe nanocomposite magnets with the core-shell structure and have revealed that the achievable \((BH)_{\text{max}}\) value of SmCo₅/α-Fe ones at 473 K is much higher than that of Nd₂Fe₁₄B/α-Fe ones. The temperature dependence of \(H_c\) for the SmCo₅/Sm₂Co₁₇ magnets also have been calculated.

Experimentally, \((BH)_{\text{max}}\) values exceeding the theoretical limit of SmCo₅ have been achieved. It has been also reported that a Sm-Co/α-Fe multi-layered thick film-magnet has a small temperature coefficient of \(H_c\), approximately −0.3%/K. These experimental results suggest the importance of Sm-Co/α-Fe multi-layered magnets, and the clarification of potential of a Sm-Co/α-Fe layered structure is needed for further investigations.

In this contribution, we calculated magnetic properties at room and high temperatures for isotropic as well as anisotropic SmCo₅/α-Fe nanocomposite magnets with a layered structure by the micromagnetic simulation.

II. SIMULATION MODEL AND METHOD

We assumed the model magnet shown in Fig. 1(a) in which SmCo₅ and α-Fe layers are stacked periodically. The simulation was carried out for the cubic region shown in Fig. 1(b) which was divided into 32,768 elements.

In anisotropic magnets, we assumed the in-plane uniaxial magnetic anisotropy for the SmCo₅ layer. The stacking periods, \(t_c\), were set to 8 and 16 nm, and the thickness ratio of SmCo₅ layer to α-Fe one was varied. An external field was applied in the in-plane direction.

The isotropic model was composed of 32 SmCo₅ cubic grains and non-anisotropic α-Fe layer. The easy directions of magnetization of SmCo₅ grains were determined by the random function so that the average of \(\cos \theta\) becomes 0.5, where \(\theta\) is the angle between the easy direction of magnetization and the applied field. The thickness ratio of SmCo₅ layer to α-Fe one was set to 1 and \(t_c\) was varied. The calculation was carried out for five model magnets prepared by different series of random numbers.

The simulation parameters of SmCo₅ and α-Fe at 300 and 473 K were reported elsewhere. Those of Nd₂Fe₁₄B were cited from Ref. 12, and shown in Table I. The detailed method of determining parameters at 473 K was also reported elsewhere. The exchange constant \(J_{\text{ex}}\) at the interface between Nd₂Fe₁₄B and α-Fe was assumed to be \(1.6 \times 10^{-3}\) J/m². \[http://dx.doi.org/10.1063/1.4861558\]

![FIG. 1. Simulation model.](Image)
the same value was assumed for $J_{sh}$ at the interface between SmCo$_5$ and $\alpha$-Fe.

### III. RESULTS AND DISCUSSION

#### A. Anisotropic SmCo$_5$/\(\alpha\)-Fe magnets

Figure 2 shows the coercivity $H_c$ of SmCo$_5$/\(\alpha\)-Fe nanocomposite magnets at 300 K as a function of the \(\alpha\)-Fe fraction $f_{Fe}$, together with the results for Nd$_2$Fe$_{14}$B/\(\alpha\)-Fe. The stacking periods $t_s$ were set at 8 and 16 nm. $H_c$ rapidly decreased with increasing $f_{Fe}$ for both the SmCo$_5$/\(\alpha\)-Fe and Nd$_2$Fe$_{14}$B/\(\alpha\)-Fe magnets. It should be noted that $H_c$ of SmCo$_5$/\(\alpha\)-Fe magnets is higher than that of Nd$_2$Fe$_{14}$B/\(\alpha\)-Fe ones for all the $f_{Fe}$ values investigated.

#### B. Isotropic SmCo$_5$/\(\alpha\)-Fe magnets

Figure 5 shows $H_c$ at 300 and 473 K as a function of $t_s$. The averaged $H_c$ values for five models and error bars were indicated. The $H_c$ vs $t_s$ curve had a broad peak and the increase in temperature shifted the peak toward right-hand side. The peak $H_c$ values at 300 and 473 K were 500 and 350 kA/m, respectively. The calculated temperature coefficients $\beta$ of $H_c$ for anisotropic and isotropic magnets were approximately $-0.20$%/K and $-0.28$%/K, respectively, which are much smaller than those for Nd-Fe-B-based magnets, approximately $-0.50$%/K. The $\beta$ value for isotropic one roughly agrees with that for the Sm-Co/\(\alpha\)-Fe multi-layered film synthesized by the pulsed laser deposition (PLD) method.

#### TABLE I. Simulation Parameters of Nd$_2$Fe$_{14}$B at 300 and 473 K.

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>$M_s$ (T)</th>
<th>$K_u$ (kJ/m$^3$)</th>
<th>$A$ ($10^{-11}$ kJ/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>1.61</td>
<td>4.5</td>
<td>0.87</td>
</tr>
<tr>
<td>473</td>
<td>1.19</td>
<td>1.64</td>
<td>0.48</td>
</tr>
</tbody>
</table>

**FIG. 2.** Coercivity $H_c$ of anisotropic SmCo$_5$/\(\alpha\)-Fe nanocomposite magnets at 300 K as a function of \(\alpha\)-Fe fraction, together with the results for Nd$_2$Fe$_{14}$B/\(\alpha\)-Fe. The stacking periods $t_s$ were set at 8 and 16 nm.

**FIG. 3.** ($BH_{\text{max}}$) of anisotropic SmCo$_5$/\(\alpha\)-Fe nanocomposite magnets at 300 K as a function of \(\alpha\)-Fe fraction together with the results for Nd$_2$Fe$_{14}$B/\(\alpha\)-Fe ones. The stacking periods were set at 8 and 16 nm.

**FIG. 4.** ($BH_{\text{max}}$) of anisotropic SmCo$_5$/\(\alpha\)-Fe nanocomposite magnets at 473 K as a function of \(\alpha\)-Fe fraction together with the results for Nd$_2$Fe$_{14}$B/\(\alpha\)-Fe ones. The stacking period was set at 8 nm.

**FIG. 5.** Coercivity $H_c$ of isotropic SmCo$_5$/\(\alpha\)-Fe nanocomposite magnets at 300 K and 473 K as a function of the stacking period, $t_s$. The averaged $H_c$ values for five models and error bars were shown in the figure. The thickness ratio of \(\alpha\)-Fe to SmCo$_5$ layers was set at 1.
approximately 300 and 250 kJ/m³, respectively. The (BH)_{max} values for Nd-Fe-B-based magnets, approximately $-0.50\%/K$.

The above results suggest that anisotropic as well as isotropic SmCo$_5$/z-Fe nanocomposite magnets with a layered structure can be used at a high temperature because of their low temperature coefficient of $H_c$ and a large (BH)$_{max}$ value at a high temperature.

IV. CONCLUSIONS

Magnetic properties of anisotropic and isotropic SmCo$_5$/z-Fe nanocomposite magnets with a layered structure were analyzed by computer simulations based on the micromagnetic theory. The obtained results are summarized as follows:

1. The (BH)$_{max}$ values of approximately 800 and 700 kJ/m³ can be achieved for the magnets at 300 and 473 K, respectively. The value at 473 K is much higher than that for Nd$_2$Fe$_14$B/z-Fe nanocomposite magnets.

2. $H_c$ of anisotropic magnets monotonically increased with reducing $t_s$, whereas the $H_c$ vs $t_s$ curves of isotropic magnets had a broad peak value between 20 and 30 nm. The behavior of $H_c$ of isotropic magnets was almost determined by the ratio of exchange energy to magnetic anisotropy one.

3. The temperature coefficient of $H_c$ for anisotropic and isotropic were approximately $-0.20\%/K$ and $-0.28\%/K$, respectively, which are much smaller than those for Nd-Fe-B-based magnets, approximately $-0.50\%/K$.

4. The (BH)$_{max}$ of isotropic magnets vs $t_s$ curves had a peak. The peak (BH)$_{max}$ values were approximately 300 and 250 kJ/m³ at 300 and 473 K, respectively.

The presence of the peak of $H_c$ can be explained by averaging effect of the magnetic anisotropy, because the reduction in the grain size increases the effective inter-grain exchange interaction and decreases the effective magnetic anisotropy. As the exchange constant in hard grains is exchange interaction and decreases the effective magnetic anisotropy, because the reduction in the grain size increases the effective inter-grain exchange energy to the magnetic anisotropy one, $\eta = J_0S/K_AV$, where $K_u$, $K_A$, and $J_0$ are the magnetic anisotropy constant, the anisotropy field, and the exchange constant of SmCo$_5$. Furthermore, $S$ and $V$ are the surface area and volume of a grain. It is clearly seen that the results at 300 and 473 K can be plotted on the same curve, which strongly suggests that $H_c$ of SmCo$_5$/z-Fe is determined by the ratio of exchange energy to magnetic anisotropy one.

Figure 7 showed (BH)$_{max}$ of isotropic magnets at 300 K and 473 K as a function of the stacking period, $t_s$. The averaged values for 5 model magnets are shown in the Figure.

The above results suggest that anisotropic SmCo$_5$/z-Fe nanocomposite magnets with a layered structure can be used at a high temperature because of their low temperature coefficient of $H_c$ and a large (BH)$_{max}$ value at a high temperature.


