

Computer simulations of the magnetic properties of Sm-Co/ α -Fe nanocomposite magnets with a core-shell structure

H. Fukunaga¹, R. Horikawa¹, M. Nakano¹, T. Yanai¹, T. Fukuzaki², K. Abe²

¹ Nagasaki University, Nagasaki 852-8521, Japan

² Samsung Yokohama Research Institute, Yokohama 230-0027, Japan

The magnetic properties of SmCo₅/ α -Fe nanocomposite magnets with a core-shell structure were computer-simulated for varying particle size L , α -Fe fraction, and temperature. The structure, consisting of a hard SmCo₅ core and a soft α -Fe shell demonstrated better magnetic properties than those of the inverse structure. The $(BH)_{\max}$ value for anisotropic magnets was approximately 800 kJ/m³ at room temperature for an L value of 6.4 nm and an α -Fe fraction of 87.5%. At 473 K, the achievable $(BH)_{\max}$ value was approximately 700 kJ/m³. These values are comparable to and higher than those for Nd₂Fe₁₄B/ α -Fe nanocomposite magnets at room temperature and 473 K, respectively, indicating a promising potential for high-temperature SmCo₅/ α -Fe nanocomposite magnets.

Index Terms—Sm-Co, α -Fe, nanocomposite, core-shell structure, $(BH)_{\max}$, coercivity

I. INTRODUCTION

Recently, high performance permanent magnets usable at high temperatures have increased in importance because of the increasing production of hybrid vehicles and electric vehicles. Because of the high Curie temperatures of Sm-Co alloys [1], a Sm-Co/ α -Fe nanocomposite magnet is a good candidate for a high performance magnet for use at high temperatures, and the synthesis of isotropic and anisotropic Sm-Co/ α -Fe nanocomposite magnets has been reported [2-5]. It is well-known that the presence of α -Fe increases the saturation magnetization and decreases the coercivity H_c [6, 7]. The high magnetocrystalline anisotropy of Sm-Co enables the presence of a large amount of α -Fe in the magnets, while necessitating a small grain size [6, 7]. Therefore, microstructural design is an important issue in developing Sm-Co/ α -Fe nanocomposite magnets. Furthermore, clarification of the potential of Sm-Co/ α -Fe nanocomposite magnets for use at high temperatures as well as room temperature is required.

The present investigation focused on SmCo₅/ α -Fe nanocomposite magnets with a core-shell structure, because a high $(BH)_{\max}$ value can be obtained when magnetically hard grains do not make contact with each other [8]. The relationship between the nanostructure and the achievable magnetic properties was estimated using micromagnetic simulations. The achievable $(BH)_{\max}$ values of SmCo₅/ α -Fe nanocomposite magnets are comparable to those for Nd₂Fe₁₄B/ α -Fe magnets at room temperature, and are much higher than those for Nd₂Fe₁₄B/ α -Fe magnets at 473 K.

II. CALCULATION MODEL

The particles illustrated in Fig. 1 were assumed for the simulation. The model particles of size L were composed of anisotropic SmCo₅ and isotropic α -Fe parts, and had a core-shell structure. Each particle was divided into 32768 cubic elements. Periodic boundary conditions were adopted in three directions so that infinitely large magnets were assumed.

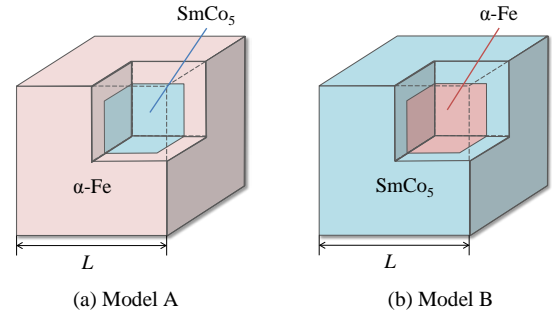


Fig. 1 Model core-shell particle structure.

III. CALCULATION METHOD

The total magnetic energy W stored in the model magnet when an external field \mathbf{H} is applied is given as

$$W = K_u^{(H)} V \sum_{i=1}^{N^3} \left\{ \frac{K_{ui}}{K_u^{(H)}} (\mathbf{u}_i \cdot \mathbf{m}_i)^2 - \sum_{j=1}^6 \left[\frac{J_{ej} S}{6K_u^{(H)} V} (\mathbf{m}_i \cdot \mathbf{m}_j) \right] - \frac{M_{si}}{K_u^{(H)}} (\mathbf{m}_i \cdot \mathbf{H}) \right\} + W_m, \quad (1)$$

where K_{ui} and M_{si} are the anisotropy constant and the saturation polarization of the i th element, respectively, and their values depend on the type of element. W_m represents the magnetostatic energy due to a local demagnetizing field. N is the total number of elements, while S and V are the surface area and volume of each element, respectively. Furthermore, \mathbf{u}_i is a unit vector in the direction of the easy axis of the i th element. \mathbf{m}_i and \mathbf{m}_j are the polarization vectors in the i th and the j th elements, respectively, and are reduced by the saturation magnetization of the corresponding element. Moreover, J_{ij} is the exchange interaction constant per unit surface area between the i th and j th elements, and has three values depending on the neighboring element type, as shown in Fig. 2.

The intra-phase exchange interaction constant J_{ss} or J_{hh} was calculated from the exchange stiffness constant A for the

TABLE I SIMULATION PARAMETERS.

	SmCo ₅		α-Fe	
	300	473	300	473
Temperature T [K]	300	473	300	473
Anisotropy constant K_u [MJ/m ³]	10.0	6.80	0.00	0.00
Saturation Polarization M_s [T]	1.00	0.95	2.15	2.09
Exchange stiffness constant A [10 ⁻¹¹ J/m]	1.20	1.09	2.50	2.36
Model size L [nm]	6.40 – 64.0			

corresponding SmCo₅ or α-Fe phase under the assumption that the element size δD is sufficiently small, as

$$J^{(i)} = A / \delta D. \quad (2)$$

The exchange constant J_{sh} at the interface between SmCo₅ and α-Fe is not known, so a value of 1.0×10^{-3} J/m² was assumed, which is approximately two thirds of the value for the α-Fe – α-Fe interface [9]

Table I shows the assumed simulation parameters at room temperature (300 K) and 473 K. The parameters at room temperature were taken from reference [1]. M_s and K_u for SmCo₅ at 200°C and M_s for α-Fe at 200°C were estimated from the declination of the curves indicated in references [10], [11], and [12], respectively. The exchange constant A at room temperature was taken from reference [1], and the constant at 473 K was estimated using the following equation [13]

$$A = cM_s(T)^2, \quad (3)$$

where M_s is the saturation polarization for SmCo₅ or α-Fe. J_{sh} was also assumed to be proportional to the average saturation polarization for SmCo₅ or α-Fe.

IV. CALCULATION RESULTS

A) Effect of the structure on demagnetization curves

A comparison of the demagnetization curves for Models A and B was carried out for various particle sizes (L) using an α-Fe fraction of approximately 50%. The magnetic properties of

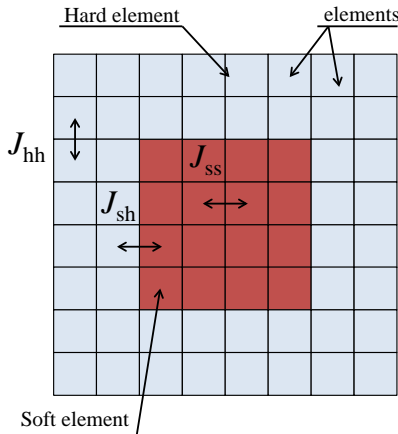


Fig.2 Exchange interaction constants between two elements. J_{ij} has three values depending on the neighboring element types.

both models significantly depended on L , as shown in Fig. 3. For example, when L was larger than 10 nm, magnetization reversal occurred incoherently. The incoherent magnetization reversals for Model B tended to be more remarkable than those for Model A. This phenomenon is explained by the fact that the magnetization reversal of the soft phase tended to occur more easily in Model B, because the soft phase was thicker than in Model A. On the other hand, as L became smaller than 10 nm, coherent magnetization reversals occurred in both models. These results suggest that Model A with a hard SmCo₅ core and a soft α-Fe shell is the better structure for obtaining superior squareness of the demagnetization curves.

B) Coercivity and $(BH)_{max}$

The magnetic properties for Model A as a function of the α-Fe fraction were next evaluated. As seen in Fig. 4, H_c at room temperature decreased with increasing α-Fe fraction for all L values. Figure 5 shows the $(BH)_{max}$ values at room temperature for the same models displayed in Fig. 4. The dotted line in the figure indicates the theoretical limit, which was calculated from the saturation polarization. The calculated $(BH)_{max}$ values had a peak for each particle size L . A $(BH)_{max}$ value of approximately 800 kJ/m³ could be obtained with an L value of 6.4 nm and an α-Fe fraction of 87.5%. We have previously reported that for Nd₂Fe₁₄B/α-Fe nanocomposite magnets, a $(BH)_{max}$ value of approximately 700 kJ/m³ is achievable for magnets with a grain-dispersed structure [8, 14], and 800 kJ/m³ is possible for magnets with a layered structure [15].

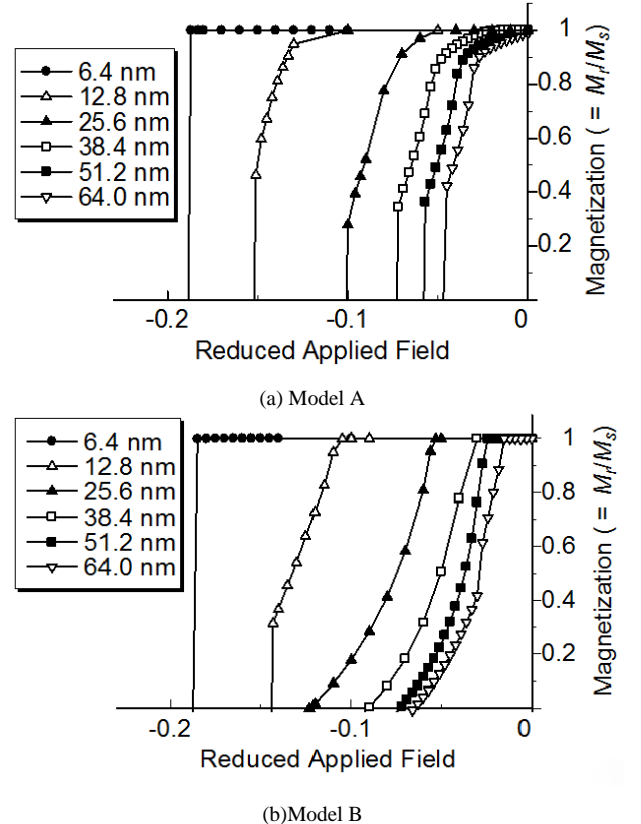


Fig. 3 Demagnetization curves at room temperature, calculated for Model A and Model B with various L values.

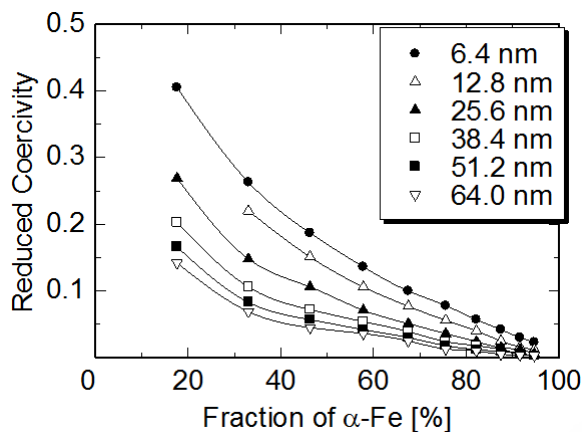


Fig. 4 Coercivity for Model A at room temperature as a function of α -Fe fraction for various L values.

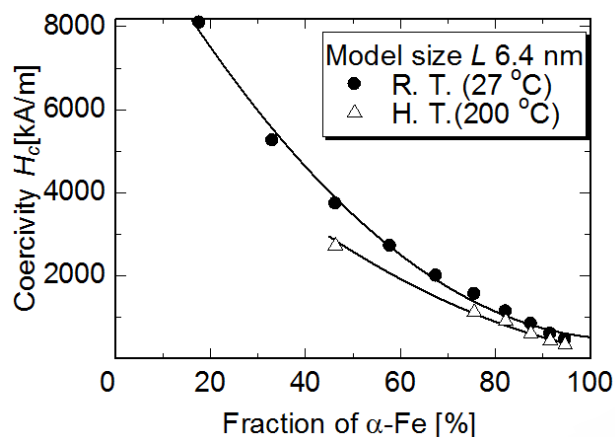


Fig. 6 Coercivity for Model A as a function of α -Fe fraction at room temperature and 473 K. The particle size L was set at 6.4 nm

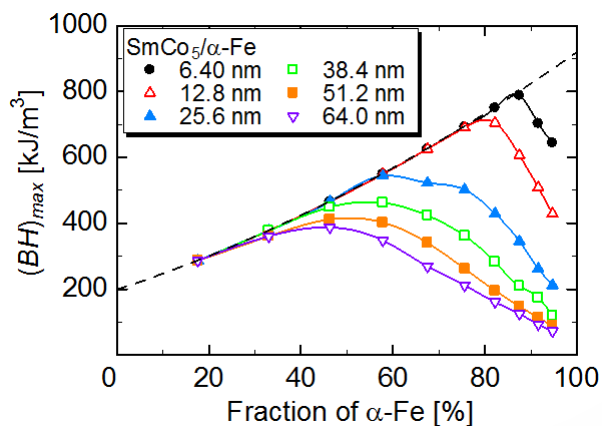


Fig. 5 $(BH)_{max}$ for Model A at room temperature as a function of α -Fe fraction for various L values.

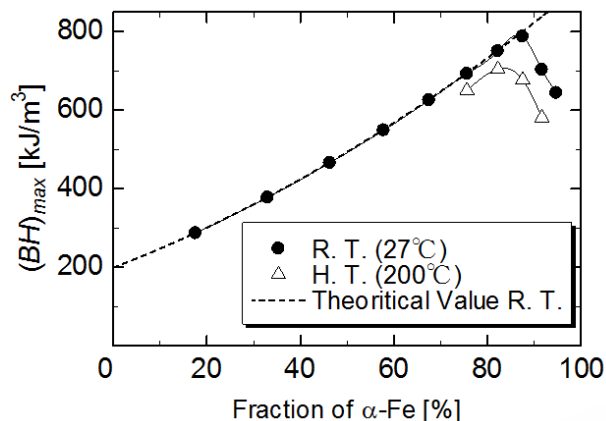


Fig. 7 $(BH)_{max}$ for Model A as a function of the fraction of α -Fe at room and 473 K. The particle size L was set at 6.4 nm. The dotted line indicates the theoretical limit calculated from the saturation polarization

Therefore, the above $(BH)_{max}$ value for $\text{SmCo}_5/\alpha\text{-Fe}$ is comparable to that for $\text{Nd}_2\text{Fe}_{14}\text{B}/\alpha\text{-Fe}$ nanocomposite magnets. The large $(BH)_{max}$ value for $\text{SmCo}_5/\alpha\text{-Fe}$ can be attributed to the large magnetic anisotropy of SmCo_5 , which enables the inclusion of a large amount of $\alpha\text{-Fe}$.

C) Temperature dependences

Although it is well-accepted that Sm-Co magnets have superior thermal stability of their magnetic properties compared with other rare-earth magnets such as Nd-Fe-B magnets, the magnetic properties of $\text{SmCo}_5/\alpha\text{-Fe}$ nanocomposite magnets have not been sufficiently investigated at high temperatures. Therefore, their magnetic properties at 473 K were calculated for various $\alpha\text{-Fe}$ fractions. In the calculations, L was fixed at 6.4 nm. As shown in Fig. 6, H_c decreased slightly by 20% due to the rise in temperature from 300 to 473 K. Figure 7 shows $(BH)_{max}$ values as a function of the $\alpha\text{-Fe}$ fraction for the same models displayed in Fig. 6. The $(BH)_{max}$ values at both 300 and 473 K exhibited peaks, and the peak $(BH)_{max}$ value at 473 K was approximately 700 kJ/m^3 for an $\alpha\text{-Fe}$ fraction of approximately 80%. As the achievable $(BH)_{max}$ value for $\text{Nd}_2\text{Fe}_{14}\text{B}/\alpha\text{-Fe}$ nanocomposite magnets with a layered structure has been reported to be approximately 500 kJ/m^3 [15], the calculated $(BH)_{max}$ value for

$\text{SmCo}_5/\alpha\text{-Fe}$ magnets suggests a promising potential for these magnets for use at high temperatures.

V. CONCLUSIONS

The magnetic properties of anisotropic $\text{SmCo}_5/\alpha\text{-Fe}$ nanocomposite magnets with a core-shell structure were analyzed by computer simulations based on micromagnetic theory. In particular, investigations of the effects of structure, particle size, and $\alpha\text{-Fe}$ fraction on the magnetic properties were carried out. The temperature dependence of the properties was also examined. The obtained results are summarized as follows:

- (1) Model A with a hard SmCo_5 core and an $\alpha\text{-Fe}$ shell had more square demagnetization curves than Model B.
- (2) A $(BH)_{max}$ value of approximately 800 kJ/m^3 could be achieved with a particle size of 6.4 nm and an $\alpha\text{-Fe}$ fraction of 87.5%. This value is comparable to that for $\text{Nd}_2\text{Fe}_{14}\text{B}/\alpha\text{-Fe}$ nanocomposite magnets.
- (3) The coercivity values were reduced by only 20% with increasing temperature from room temperature to 473 K.

- (4) Maximum $(BH)_{\max}$ values of approximately 700 kJ/m^3 could be obtained at 473 K with a particle size of 6.4 nm and an α -Fe fraction of approximately 80%. This value is much higher than that reported for $\text{Nd}_2\text{Fe}_{14}\text{B}/\alpha\text{-Fe}$ nanocomposite magnets, which suggests a promising potential for $\text{SmCo}_5/\alpha\text{-Fe}$ nanocomposite magnets for use at high temperatures.

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