Magnetic properties of isotropic and anisotropic $SmCo_5$/α-Fe nanocomposite magnets with a layered structure simulated by micromagnetic theory

R. Horikawa,[a)] H. Fukunaga, M. Nakano, and T. Yanai
Graduate school of Engineering, Nagasaki University, Nagasaki, Nagasaki 852-8521, Japan

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Magnetic properties of anisotropic and isotropic $SmCo_5$/α-Fe nanocomposite magnets with a layered structure were computer-simulated with varying the stacking period, the α-Fe fraction, and temperature. The $(BH)_{max}$ values of approximately 800 and 700 kJ/m^3 were achieved for anisotropic magnets at 300 and 473 K, respectively. These values roughly agree with results for $SmCo_5$/α-Fe with a core-shell structure, and the value at 473 K is much higher than that of $Nd_2Fe_{14}B$/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 $(BH)_{max}$ values were approximately 300 and 250 kJ/m^3 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.
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I. INTRODUCTION

Nanocomposite magnets are hopeful candidates for next generation magnets. Because of high Curie temperatures of Sm-Co alloys,[1] 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.[2,3] 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 strutures.[4–7] We have already calculated the temperature dependence of the magnetic properties of $SmCo_5$/α-Fe nanocomposite magnets with the core-shell structure and have revealed that the achievable $(BH)_{max}$ value of $SmCo_5$/α-Fe ones at 473 K is much higher than that of $Nd_2Fe_{14}B$/α-Fe ones.[3] The temperature dependence of H_c for the $SmCo_5/Sm_2Co_{17}$ magnets also have been calculated.[8]

Experimentally, $(BH)_{max}$ values exceeding the theoretical limit of $SmCo_5$ have been achieved.[9,10] 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.[11] 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 $SmCo_5$/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 $SmCo_5$ 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 $SmCo_5$ layer. The stacking periods, t_s, were set to 8 and 16 nm, and the thickness ratio of $SmCo_5$ layer to α-Fe one was varied. An external field was applied in the in-plane direction.

The isotropic model was composed of 32 $SmCo_5$ cubic grains and non-anisotropic α-Fe layer. The easy directions of magnetization of $SmCo_5$ grains were determined by the random function so that the average of $\cos\theta$ becomes 0.5, where θ is the angle between the easy direction of magnetization and the applied field. The thickness ratio of $SmCo_5$ layer to α-Fe one was set to 1 and t_s was varied. The calculation was carried out for five model magnets prepared by different series of random numbers.

The simulation parameters of $SmCo_5$ and α-Fe at 300 and 473 K were reported elsewhere.[11] Those of $Nd_2Fe_{14}B$ were cited from Ref. 12, and shown in Table I. The detailed method of determining parameters at 473 K was also reported elsewhere.[11] The exchange constant J_{sh} at the interface between $Nd_2Fe_{14}B$ and α-Fe was assumed to be 1.6×10^{-3} J/m^2,[13] and

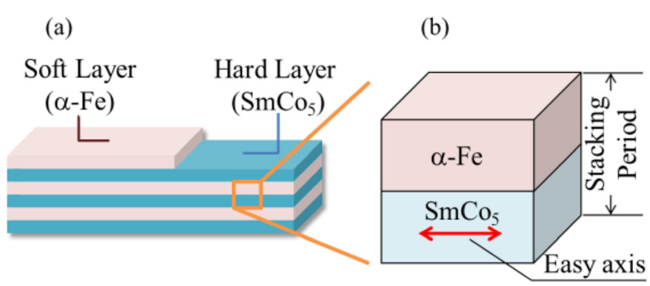

FIG. 1. Simulation model.

[a)]Author to whom correspondence should be addressed. Electronic mail: bb52112234@cc.nagasaki-u.ac.jp. Fax: +81-95-846-7379.

TABLE I. Simulation Parameters of $Nd_2Fe_{14}B$ at 300 and 473 K.

Temperature (K)	M_s (T)	K_u (kJ/m^3)	A (10^{-11} kJ/m)
300	1.61	4.5	0.87
473	1.19	1.64	0.48

the same value was assumed for J_{sh} at the interface between $SmCo_5$ and α-Fe.

III. RESULTS AND DISCUSSION

A. Anisotropic $SmCo_5$/α-Fe magnets

Figure 2 shows the coercivity H_c of $SmCo_5$/α-Fe nanocomposite magnets at 300 K as a function of the α-Fe fraction f_{Fe}, together with the results for $Nd_2Fe_{14}B$/α-Fe. The stacking periods t_s were set at 8 and 16 nm. H_c rapidly decreased with increasing f_{Fe} for both the $SmCo_5$/α-Fe and $Nd_2Fe_{14}B$/α-Fe magnets. It should be noted that H_c of $SmCo_5$/α-Fe magnets is higher than that of $Nd_2Fe_{14}B$/α-Fe ones for all the f_{Fe} values investigated.

Figure 3 shows $(BH)_{max}$ of anisotropic $SmCo_5$/α-Fe at 300 K as a function of f_{Fe}, together with the results for $Nd_2Fe_{14}B$/α-Fe ones. It is clearly seen that the decrease in t_s enables us to increase in f_{Fe}. The available amount of α-Fe also increases by selecting $SmCo_5$ instead of $Nd_2Fe_{14}B$ as a magnetically hard phase, which can be attributed to the large

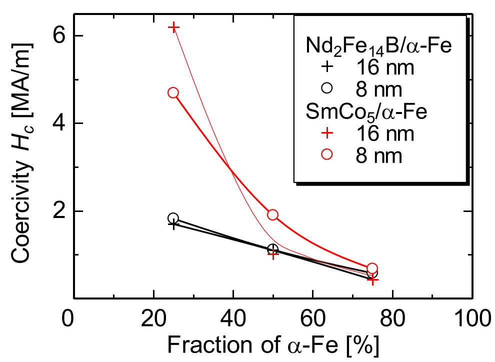

FIG. 2. Coercivity of anisotropic $SmCo_5$/α-Fe nanocomposite magnets at 300 K as a function of α-Fe fraction, together with results for $Nd_2Fe_{14}B$/α-Fe ones. The stacking periods were set at 8 and 16 nm.

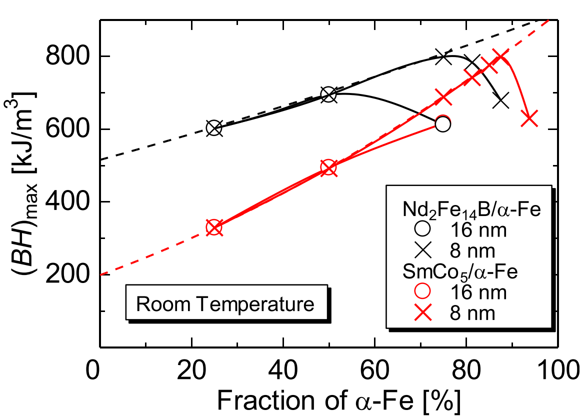

FIG. 3. $(BH)_{max}$ of anisotropic $SmCo_5$/α-Fe nanocomposite magnets at 300 K as a function of α-Fe fraction together with results for $Nd_2Fe_{14}B$/α-Fe ones. The stacking periods were set at 8 and 16 nm.

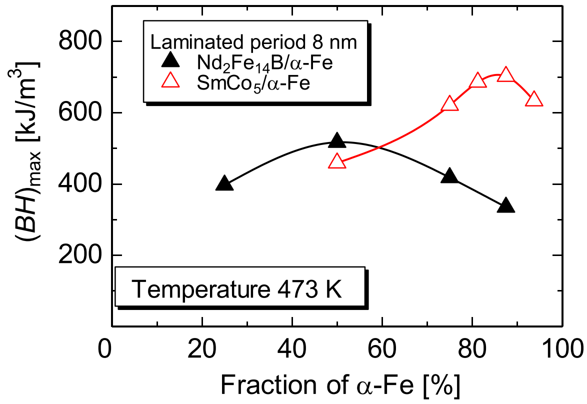

FIG. 4. $(BH)_{max}$ of anisotropic $SmCo_5$/α-Fe nanocomposite magnets at 473 K as a function of the fraction of α-Fe together with results for $Nd_2Fe_{14}B$/α-Fe ones. The stacking period was set at 8 nm.

magnetic anisotropy constant of $SmCo_5$. Resultantly, the highest $(BH)_{max}$ value of $SmCo_5$/α-Fe magnets, 800 kJ/m^3, was obtained at $f_{Fe} = 85\%$ and $t_s = 8$ nm. This value roughly agrees with results for $SmCo_5$/α-Fe with a core-shell structure.[11]

The $(BH)_{max}$ values at 473 K was shown in Fig. 4 as a function of f_{Fe}, together with results for $Nd_2Fe_{14}B$/α-Fe ones. In $SmCo_5$/α-Fe magnets, the achievable $(BH)_{max}$ value at 473 K was approximately 700 kJ/m^3 at $f_{Fe} = 80\%$, which is much higher than that of $Nd_2Fe_{14}B$/α-Fe, approximately 500 kJ/m^3.

B. Isotropic $SmCo_5$/α-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 are 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 β 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 β value for isotropic one roughly agrees with that for the Sm-Co/α-Fe multi-layered film synthesized by the pulsed laser deposition (PLD) method.[14]

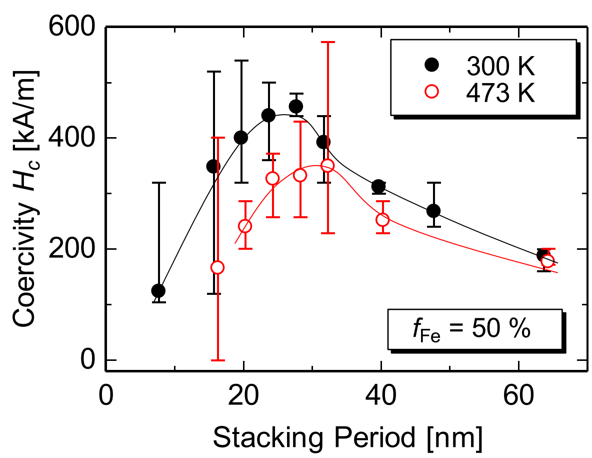

FIG. 5. Coercivity H_c of isotropic $SmCo_5$/α-Fe nanocomposite magnets at 300 K and 473 K as a function of the stacking period, t_s. The averaged H_c values for five models and error bars were shown in the figure. The thickness ratio of α-Fe to $SmCo_5$ layers was set at 1.

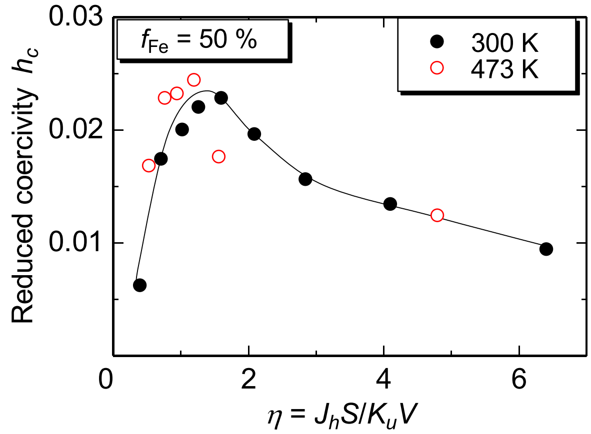

FIG. 6. Reduced coercivity, h_c ($= H_c/H_A$), as a function of η ($= J_hS/K_uV$), where K_u and K_A are the magnetic anisotropy constant and anisotropy field of $SmCo_5$, and S and V are the surface area and volume of a grain. Furthermore, J_h is the exchange constant of $SmCo_5$. The explanation about η is in the text.

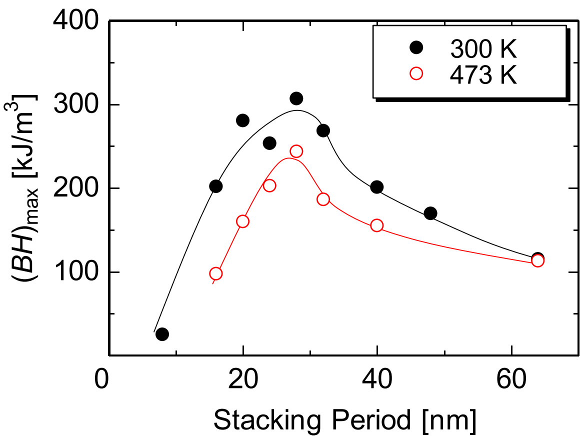

FIG. 7. $(BH)_{max}$ of isotropic $SmCo_5/\alpha$-Fe nanocomposite magnets at 300 K and 473 K as a function of the stacking period, t_s. The averaged values for 5 model magnets are shown in the Figure.

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.[15,16] As the exchange constant in hard grains is the dominant exchange one determining magnetic properties of nanocomposite magnets,[2,3] we re-plotted the reduced coercivity h_c ($=H_c/K_A$) in Fig. 6 as a function of the ratio of exchange energy to the magnetic anisotropy one, η ($= J_hS/K_uV$), where K_u, K_A, and J_h 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 $SmCo_5/\alpha$-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 t_s. The $(BH)_{max}$ values for five models were indicated. The $(BH)_{max}$ vs t_s curves at 300 and 473 K had a peak. The peak value at 300 and 473 K were approximately 300 and 250 kJ/m^3, respectively. The $(BH)_{max}$ value at 300 K agrees roughly with that for a dispersed $Nd_2Fe_{14}B/\alpha$-Fe nanocomposite magnet.[3]

IV. CONCLUSIONS

Magnetic properties of anisotropic and isotropic $SmCo_5/\alpha$-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/m^3 can be achieved for the magnets at 300 and 473 K, respectively. The value at 473 K is much higher than that for $Nd_2Fe_{14}B/\alpha$-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/m^3 at 300 and 473 K, respectively.

The above results suggest that anisotropic as well as isotropic $SmCo_5/\alpha$-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.

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