Effect of magnetic properties of soft magnetic phase on the energy product of an exchange-spring magnet*

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Research on exchange-spring magnets has focused on the microstructures of the materials. However, research has seldom been concerned with the effect of magnetic properties of soft magnetic phase on the energy product of an exchange-spring magnet. In this paper, a simple one-dimensional numerical simulation is used to investigate this effect in a $Nd_2Fe_{14}B$-based exchange-spring magnet. The results reveal that the larger the anisotropy constant, the stronger the exchange coupling, and the higher the magnetization of the soft magnetic phase, the larger the energy product of an exchange-spring magnet. This provides evidence for choosing a soft magnetic phase in an exchange-spring magnet.

Keywords: exchange-spring magnets, numerical simulation

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1. Introduction

The energy product is the most important parameter for a permanent magnet. In order to improve the energy product, exchange-spring magnets have been extensively studied in the last two decades since it was discovered by Coehoorn *et al*.[1] An exchange-spring magnet has a relatively low content of rare earth, which makes the magnet cheaper and more thermally stable. The mechanism of an exchange-spring magnet was first proposed by Kneller and Hawig.[2] The idea is that hard and soft phases in an exchange-spring magnet can be exchange-coupled in an appropriate nanostructure in such a way that the exchange-spring magnet exhibits hard magnetic properties. Skomski and Coey[3] showed that the length scale of the soft phase should be on the order of the domain wall width of the hard phase (a few nanometers) and they suggested that it should be possible to achieve an energy product in excess of 1 MJ/m^3 in an optimized hard/soft nanocomposite. This theoretically-predicted giant energy product is about twice as high as the present highest recorded energy product found in $Nd_2Fe_{14}B$. However, the typical energy product achieved in an exchange-spring magnet by experimental efforts in the past 20 years is 160 kJ/m^3, which is far below the expected value of 1 MJ/m^3.[4–7] The huge gap may be due to the random easy axis orientation of hard phase nanocrystallines and non-uniform microstructures in experimental samples, whereas the easy axis is perfectly and fully aligned and the microstructure is uniform in the theoretical model. However, besides the easy axis orientation degrees of hard phase nanocrystallines and the uniformity of the microstructure, there are still some other considerations to take into account to optimize the energy product for an exchange-spring magnet. For example, the combination of hard and soft magnetic materials should be optimized to obtain the best energy product for an exchange-spring magnet. So far, the researches based on experiments and models have mainly focused on the effect of microstructure and exchange coupling on magnetic properties of an exchange-spring magnet. Although some papers mentioned that the optimized soft magnetic phase might improve the magnets,[8–11] no report has focused on the effect of the magnetic properties of a soft magnetic phase on the energy product of an exchange-spring magnet. Because $Nd_2Fe_{14}B$ has the highest recorded energy product, the effect of magnetic properties of a soft magnetic phase on the energy product of an exchange-spring magnet based on $Nd_2Fe_{14}B$ is investigated by a one-dimensional model[12,13] in this paper.

2. Model

The one-dimensional model is composed of the trilayer structure which is made up of a hard magnetic layer/a soft magnetic layer/a hard magnetic layer. The trilayer structure is shown in Fig. 1. The easy axes of the hard layers and soft layer are aligned along the x axis, and an external magnetic field H is also applied along the x axis. The trilayer structure is the most effective structure for an exchange-spring magnet because the exchange-coupling interface between hard and soft magnetic phases is the largest in this structure. The demagnetizing field can be neglected in the trilayer structure, which benefits the magnetic properties of exchange-spring magnets. Therefore, the investigation can focus on the material parameters rather

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than the structures. In this model, the anisotropy energy, exchange coupling energy, and Zeeman energy are considered.

$$E = -\sum_{i=1}^{N-1} \frac{a_i A_{i,i+1}}{a_i^2} \cos(\theta_i - \theta_{i+1}) - \sum_{i=1}^{N} a_i K_i \cos^2(\theta_i) - \sum_{i=1}^{N} a_i H M_i \cos(\theta_i - \theta_H), \quad (1)$$

where $A_{i,i+1}$ is the exchange coupling constant between the adjacent atomic spins, K_i is the anisotropy constant, M_i is the magnetization, a_i is the atom distance, θ_i is the angle between the atomic spin and the x axis, E is the magnetic energy per unit area of the trilayer structure, H is the applied magnetic field, i is the atomic layer number which is numbered from 1 to N in consecutive order along the z axis.

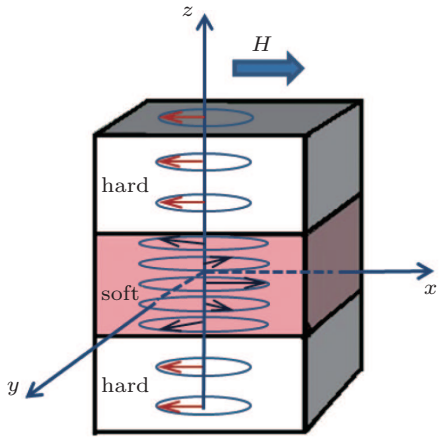


Fig. 1. (color online) Trilayer structure in one-dimensional model.

The hard layer parameters are taken from $Nd_2Fe_{14}B$ as follows:[14,15] $A_h = 0.77 \times 10^{-11}$ J/m, $K_h = 4.3 \times 10^6$ J/m^3, $M_h = 1.28 \times 10^6$ A/m, and $a_h = 2$ Å. The subscripts h and s denote hard and soft magnetic phases. The thickness of the hard layer should be no thinner than 10 nm, otherwise the hard layer shows virtually no hard magnetic properties according to our experience. For simplifying the calculation, the magnetization and atom distance of the soft layer are kept constant at 1.7×10^6 A/m and 2 Å, respectively. A_s/a_s^2 and K_s vary from 2.5×10^7 J/m^3 to 2.5×10^9 J/m^3 and from 1×10^2 J/m^3 to 1.3×10^6 J/m^3, respectively. The exchange coupling constant between the hard and soft magnetic layers is assumed to be the average exchange coupling constant value of the hard and soft magnetic layers.

3. Results and discussion

In order to optimize the energy product $(BH)_{max}$ for the $Nd_2Fe_{14}B$-based exchange-spring magnets, the dependences of $(BH)_{max}$ on thickness of hard and soft magnetic layers are investigated and the results are shown in Fig. 2. The theoretical curves are given by the following equation:[8]

$$(BH)_{max} = \mu_0 M_s^2/4, \quad (2)$$

where M_s is the saturation magnetization of the exchange-spring magnet and μ_0 is the vacuum permeability. The theoretical $(BH)_{max}$ gives the maximum limitation for the magnet. The preconditions for the theoretical $(BH)_{max}$ are the ideal square M–H loop and magnetization coercivity $\geq \mu_0 M_s/2$. The results show that $(BH)_{max}$ increases with the decrease of the thickness of the hard layer . It is due to the fact that the magnetization of the exchange-spring magnet increases with the decrease of the thickness of the hard layer. Because the thickness of the hard layer is no less than 10 nm, the best calculated $(BH)_{max}$ should be obtained when the thickness of the hard layer is 10 nm. The dependence of calculated $(BH)_{max}$ on the thickness of the soft layer shows a peak where the calculated $(BH)_{max}$ curve just breaks away from the theoretical $(BH)_{max}$ curve. The main reason for the difference between theoretical and calculated $(BH)_{max}$ curves is the calculated coercivity $< \mu_0 M_s/2$ which fails to meet the precondition for the theoretical $(BH)_{max}$ curve. The calculated $(BH)_{max}$ increases with the augment of the thickness of the soft layer until the peak point on the calculated $(BH)_{max}$ curve is reached. It may be due to the fact that the magnetization of the exchange-spring magnet increases with the augment of the thickness of the soft layer. The calculated $(BH)_{max}$ decreases with the increase of the thickness of the soft layer after the peak point on the calculated $(BH)_{max}$ curve has been reached. This may be due to the fact that the coercivity decreases below $\mu_0 M_s/2$ with the increase of the thickness of the soft layer. The best calculated $(BH)_{max}$ can be obtained by a trade off between magnetization and coercivity.

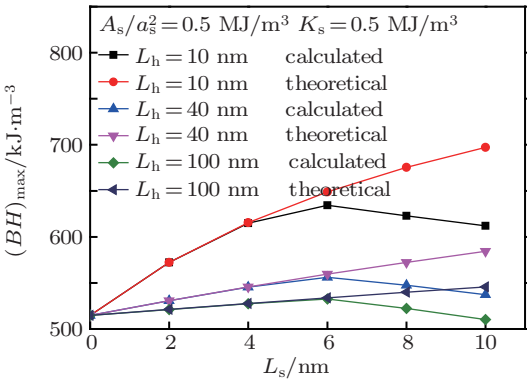


Fig. 2. (color online) Dependences of the calculated $(BH)_{max}$ and the theoretical $(BH)_{max}$ on the thickness of the soft and hard layer. The theoretical $(BH)_{max}$ is calculated from Eq. (2).

The values of best $(BH)_{max}$ are calculated by optimizing the thickness values of the hard and soft magnetic layers for various values of A_s/a_s^2 and K_s and shown in Fig. 3. Figure 3 shows that the best calculated value of $(BH)_{max}$ increases with A_s/a_s^2 and K_s increasing. This may be due to the fact that the coercivity increases with A_s/a_s^2 and K_s increasing and it may maximize the $(BH)_{max}$ if the increased coercivity is larger than $\mu_0 M_s/2$. The calculated $(BH)_{max}$ hardly

changes with A_s/a_s^2 when A_s/a_s^2 is larger than 1000 MJ/m^3 or $K_s \geqq 0.7$ MJ/m^3. In order to understand the results, the phase structures of the calculated magnets are shown in Fig. 4. Figure 4 shows that the best $(BH)_{max}$ can be expected from the single soft layer with a larger K_s. However, in this case, the soft layer cannot be regarded as a real soft material because the K_s is too large to be a conventional soft material. The best $(BH)_{max}$ can be expected from the exchange-coupled hard/soft layer structure with a small K_s. Along the boundary line between the soft layer only and exchange-coupled hard–soft layers, K_s increases with the augment of A_s/a_s^2. In order to understand the results shown in Fig. 4, figure 5 displays the plots of the calculated $(BH)_{max}$ versus the soft layer thickness for various values of K_s and A_s/a_s^2. In the case of large K_s ($= 1$ MJ/m^3), the calculated $(BH)_{max}$ increases with the augment of the thickness of the soft layer L_s no matter whether the value of A_s/a_s^2 is large (500 MJ/m^3) or small (50 MJ/m^3). It indicates that the value of best $(BH)_{max}$ can be obtained from the single soft layer ($L_s = \infty$) in the case of a soft layer with a large value of K_s. This is due to the fact that the large K_s can make the coercivity larger than $\mu_0 M_s/2$, which makes the $(BH)_{max}$ of the single soft layer maximized. In the case of small K_s ($= 0.2$ MJ/m^3), the calculated $(BH)_{max}$ shows a peak with a maximum value no matter whether the value of A_s/a_s^2 is large (500 MJ/m^3) or small (50 MJ/m^3). It indicates that the best $(BH)_{max}$ can be obtained from the exchange-coupled hard/soft layer structure with an optimized soft layer thickness in the case of the soft layer with small K_s. This is due to the fact that the soft layer with small K_s needs the exchange coupled hard layer to enhance the coecivity above $\mu_0 M_s/2$, which may maximize the $(BH)_{max}$. In the case of medium K_s ($= 0.5$ MJ/m^3 or 0.56 MJ/m^3), the calculated $(BH)_{max}$ shows a peak when L_s is around 10 nm. However, when the soft layer thickness increases further, the calculated $(BH)_{max}$ increases and the single soft layer ($L_s = \infty$) has a maximum $(BH)_{max}$ for the case of small A_s/a_s^2 (50 MJ/m^3). The peak value is the maximum calculated value of $(BH)_{max}$ for the case of large A_s/a_s^2 (500 MJ/m^3). The peak shows that the soft layer with medium K_s needs the hard layer to enhance the coercivity above $\mu_0 M_s/2$ when the thickness of the soft layer is small. When L_s is large, the reason for the increasing of calculated $(BH)_{max}$ with L_s may be that the coercivity slightly decreases with the increase of L_s and $\mu_0 M_s$ obviously increases with the augment of L_s, thereby leading to the increase of calculated $(BH)_{max}$ with the increase of L_s. In the case of large A_s/a_s^2 (500 MJ/m^3), the coercivity is large compared with that in the case of small A_s/a_s^2 (50 MJ/m^3). The tendency of coercivity decreasing with L_s in the case of large A_s/a_s^2 (500 MJ/m^3) is more obvious than that in the case of small A_s/a_s^2 (50 MJ/m^3). $\mu_0 M_s$ in the case of large A_s/a_s^2 (500 MJ/m^3) increases with the augment of L_s as much as that in the case of small A_s/a_s^2 (50 MJ/m^3). It leads to the relatively obvious increasing of calculated $(BH)_{max}$ with the increase of L_s in the case of small A_s/a_s^2 (50 MJ/m^3). Therefore, the single soft layer ($L_s = \infty$) has the maximum calculated value of $(BH)_{max}$ in the case of small A_s/a_s^2 (50 MJ/m^3). However, the hard/soft layer structure with something like a 10-nm soft layer has a maximum calculated value of $(BH)_{max}$ in the case of large A_s/a_s^2 (500 MJ/m^3).

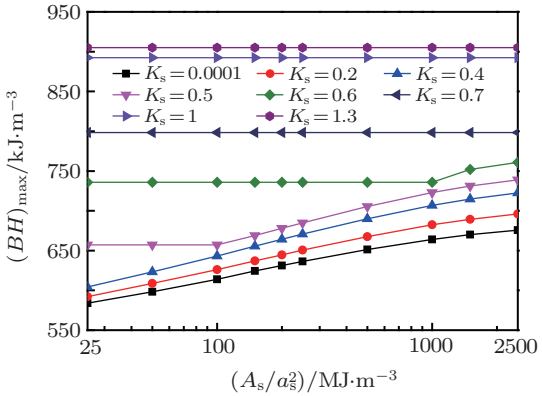


Fig. 3. (color online) Plots of calculated $(BH)_{max}$ versus A_s/a_s^2 for various values of K_s. (K_s is in unit MJ/m^3).

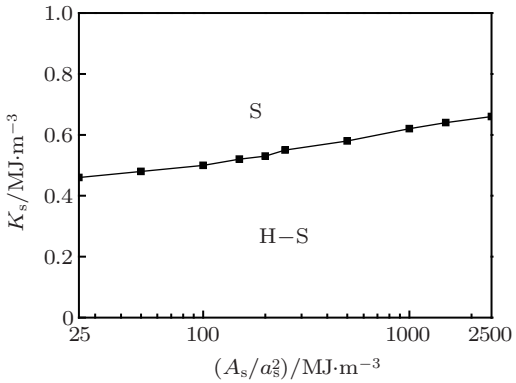


Fig. 4. Phase structures of the calculated magnet for various values of A_s/a_s^2 and K_s. S and H–S denote soft layer only and exchange-coupled hard–soft layer, respectively.

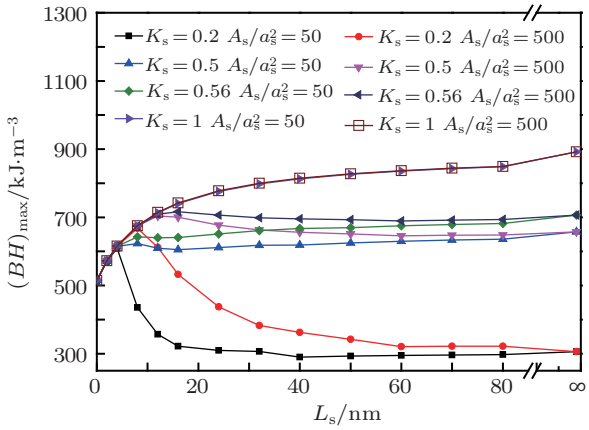


Fig. 5. (color online) Plots of calculated $(BH)_{max}$ versus soft layer thickness for various values of K_s and A_s/a_s^2 (K_s and A_s/a_s^2 are both in unit MJ/m^3).

For conventional soft materials, the values of A_s/a_s^2 are around several hundred MJ/m^3 and the values of K_s range from 0 to several 10^5 J/m^3. Therefore, the best $(BH)_{max}$ for a conventional soft material should be expected from the exchange-coupled hard–soft composite magnet according to Fig. 4. Figure 3 shows that the best $(BH)_{max}$ hardly increases with the augment of A_s/a_s^2 when A_s/a_s^2 is larger than 1000 MJ/m^3. However, figure 6 shows that the best $(BH)_{max}$ dramatically increases with the augment of K_s when K_s is several 10^5 J/m^3. This result indicates that the improving of K_s is more important than the improving of A_s/a_s^2 for the conventional soft material. The coercivity of the layer structure increases with the augment of K_s. The best $(BH)_{max}$ can be obtained according to Eq. (2) when the coercivity is larger than $\mu_0 M_s/2$. However, the further increasing of coercivity cannot increase $(BH)_{max}$ value beyond the theoretical value $\mu_0 M_s^2/4$. Therefore, $(BH)_{max}$ value increases with the augment of K_s when K_s is less than 1.0 MJ/m^3, and it is saturated when K_s is larger than 1.5 MJ/m^3.

In our calculation, the magnetization of the soft material is kept constant. In order to investigate the soft material magnetization dependences of the $(BH)_{max}$ of exchange-spring magnets, the best values of $(BH)_{max}$ are calculated for different conventional soft materials/$Nd_2Fe_{14}B$ combinations. The results shown in Table 1 indicate that the best value of $(BH)_{max}$ is strongly dependent on the magnetization of the soft material.

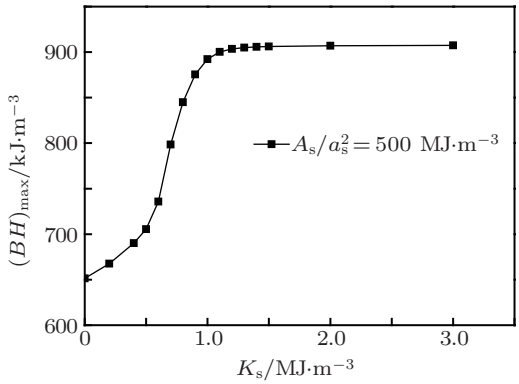


Fig. 6. Calculated $(BH)_{max}$ as a function of soft magnetic material anisotropy constant K_s.

Table 1. Calculated values of $(BH)_{max}$ for conventional soft materials/$Nd_2Fe_{14}B$ exchange-spring magnets. The parameters of conventional soft materials are adopted from Refs. [16], [14], and [11].

Soft magnetic materials	K_s/(MJ/m^3)	M_s/(MA/m)	A_s/(10^{-12} J/m)	$(BH)_{max}$/(kJ/m^3)	The soft layer thickness for the best $(BH)_{max}$/nm
Co	0.43	1.398	26	570.39	16.4
Fe	0.046	1.71	25	662.38	7.2
Fe_{65} Co_{35}	0.311	1.93	36	775.73	9.6

Our results can also be verified by previous experimental work. The experimental results[17] on SmCo/Fe show that annealing SmCo/Fe film can make Co atoms in a SmCo layer diffuse into a Fe layer and becomes SmCo/FeCo film leading to an increase of $(BH)_{max}$ value of the film. The increased $(BH)_{max}$ is due to the large magnetization and the large magnetic anisotropy constant of FeCo.

4. Summary

The best $(BH)_{max}$ is calculated by a one-dimensional model for the $Nd_2Fe_{14}B$-based exchange-spring magnets with various soft magnetic materials. The results show that the magnetization of soft magnetic material is the most important factor for maximizing the $(BH)_{max}$ of an exchange-spring magnet and the anisotropy constant of the soft magnetic material is also more important for improving $(BH)_{max}$ than exchange-coupling.

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