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Effect of α-Fe Content on the Magnetic Properties of MnBi/α-Fe Nanocomposite Permanent Magnets by Micro-magnetic Calculation

Y. Q. Li[1], M. Yue[1]*, J. H. Zuo[1], D. T. Zhang[1], W. Q. Liu[1], J. X. Zhang[1], Z. H. Guo[2], and W. Li[2]

[1]*College of Materials Science and Engineering, Beijing University of Technology, Beijing 100124, China*
[2]*Division of Functional Materials, Central Iron and Steel Research Institute, Beijing 100081, China*

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A finite element model was built for MnBi/α-Fe nanocomposite permanent magnets, and the demagnetization curves of the magnets were simulated by micro-magnetic calculation. The microstructure of the cubic model is composed of 64 irregular grains with an average grain size of 20 nm. With the volume fraction of soft magnetic phase (*t* vol. %) ranged from 5 to 20 vol. %, both isotropic and anisotropic nanocomposite magnets show typical single-phase permanent magnets behavior in their demagnetization curves, illustrating good intergranular exchange coupling effect between soft and hard magnetic phases. With the increase of volume fraction of soft magnetic phase in both isotropic and anisotropic magnets, the coercive force of the magnets decreases monotonically, while the remanence rises at first to a peak value, then decreases. The optimal values of maximum energy products of isotropic and anisotropic magnets are 84 and 200 kJ/m^3, respectively. Our simulation shows that the MnBi/α-Fe nanocomposite permanent magnets own excellent magnetic properties and therefore good potential for practical applications.

Keywords : MnBi/α-Fe nanocomposite permanent magnets, micromagnetic simulation coercive force, remanence, maximum energy products

1. Introduction

Recently, with respect to the resource limitation and high cost of special rare earth elements such as Nd and Dy, rare earth less or rare earth free permanent magnets have drawn increasing attention. Among the current low cost permanent magnets, MnBi-based magnets are competitive due not only to their high anisotropy field, but to their positive temperature coefficient of coercive force at elevated temperature. The low temperature phase (LTP) of MnBi belongs to hexagonal NaAs-type crystal structure, and it bears magnetic anisotropic field as high as 5 T. Moreover, LTP MnBi magnets exhibit a positive coercivity temperature coefficient up to 540 K [1]. The main barrier to get high maximum energy products in MnBi magnets is the low saturation magnetization of 0.78 T [2] at room temperature, which restricts the practical application of the magnets.

Nanocomposite permanent magnetic materials are mixed by hard magnetic phase with high magnetocrystalline anisotropy and soft magnetic phase with high saturation magnetization in nanoscale. The optimal magnetic properties can be acquired via ferromagnetic coupling effect between the grains of the two phases. Schrefl [3] have analyzed and calculated the demagnetization curve of the nanocomposite permanent magnet mixed with RFe (R is rare earth) compound and α-Fe by micro-magnetic finite element method (FEM), and the results showed that the properties of nanocomposite permanent magnets was sensitive to the content and the grain size of the soft phase. Skomski and Coey [4] put forward an anisotropic micro-magnetic model, and the maximum energy products of $Sm_2Fe_{17}N_3/Fe_{65}Co_{35}$ nanocomposite permanent magnet can reach the value of 1090 kJ/m^3. Therefore, it is expected to get high maximum energy products in new magnets by putting MnBi and α-Fe together in nanoscale.

In our previous works [5], the simulation model of MnBi/α-Fe nanocomposite permanent magnets consisting of spherical fourteen faces unit of hard phase grains and the soft matrix phase was made by micro-magnetism finite element model. By means of FEM, the magnetic properties of the magnets were evaluated and the value of maximum

*Corresponding author: Tel: +86-010-6739-1760
Fax: +86-010-6739-1760, e-mail: yueming@bjut.edu.cn

energy product reaching 322 kJ/m^3 for anisotropic sample. However, it is hard to control the hard magnetic phase size and the ideal distribution of the two phases in experiment.

In this paper, by building the model of random distribution of two phase grains, the demagnetization curves of MnBi/α-Fe nanocomposite permanent magnets were calculated by FEM. Effect of α-Fe content on the magnetic properties of MnBi/α-Fe nanocomposite permanent magnets was investigated since the previous calculation of nanocompostie magnets [6-11] have showed that the magnetic properties was deeply influenced by the content of the soft phase.

2. Simulation Method

Magnetic properties of nanocomposite magnets is strongly depended on their microstructure, only ideal microstructure can guarantee complete exchange-coupling effect between the soft and hard magnetic phases to obtain high magnetic properties. It should be pointed out that the exchange-coupling effect only takes place in a certain range of size, and that is almost twice as much as the thickness of Bloch wall [12]. For MnBi alloy, the thickness of Bloch wall can be calculated by the formula (1).

$$L_{MnBi} = \pi(A/K_1)^{1/2} = 10.5 \text{ nm} \quad (1)$$

In the formula, A is the integral exchange constant and K_1 is the magnetocrystalline anisotropy. In the MnBi/α-Fe nanocomposite, the grain size of the α-Fe can't scale out twice the thickness of Bloch wall to ensure exchange-coupling effect. As is known to all, the exchange-coupling effect gradually weakens from the contact area of the two phases to the center of the soft phase.

Schrefl *et al.*'s simulation model [3] was formed by 64 irregular grains of soft and hard magnetic phases that were randomly distributed in the model. It may cause the condition that two single soft phase grains are contacted together, and then forms a wide range of soft phase area in the simulation model. In the demagnetization process, magnetic reversal occurred easily in this area, and destroyed the magnetic properties. In our work, the simulation model (as shown in Fig. 1) is similar to Schrefl's model except that all the grains of soft magnetic phases are not in direct contact with each other. The distribution of the grain size was shown in Fig. 2. The particles as small as possible are chosen as the soft phase; however, large size grains over 21 nm will appear in our model if the content of the soft phase reach 20 vol. %. In this paper, The relevant material parameters are taken from Ref. 13 and 14, namely, saturated magnetization, the obtained maximum value of Magnetization with the increasing the magnetic field, J_s^{MnBi} = 0.78 T, J_s^{Fe} = 2.15 T; magnetocrystalline anisotropic constant, which is used to measure the strength of the magnetocrystalline anisotropy, K_1^{MnBi} = 0.91 MJ/m^3, K_1^{Fe} = 0.046 MJ/m^3; integral exchange constant, which is a constant used to calculate exchange energy, $A^{MnBi} = 1.0 \times 10^{-11}$ J/m, $A^{Fe} = 2.5 \times 10^{-11}$ J/m.

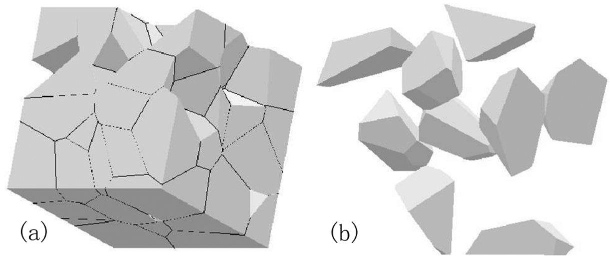

Fig. 1. The microstructure of hard (a), and soft (b) magnetic phases in simulation model with the content of α-Fe, *t* = 10 vol. %.

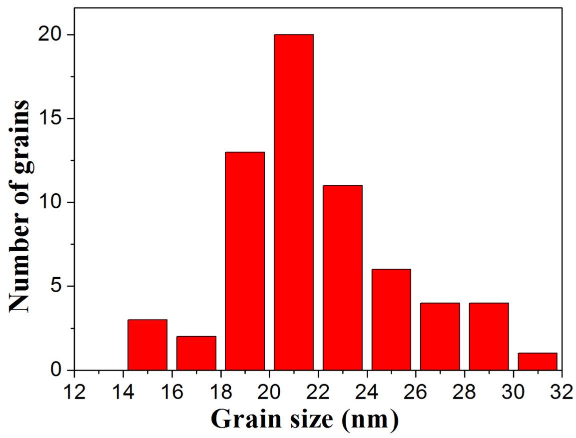

Fig. 2. (Color online) The distribution of grain size in the simulation model with the content of α-Fe, *t* = 10 vol. %.

3. Results and Discussion

3.1. Magnetic Properties of Isotropic Magnets

Figure 3 shows the demagnetization curves of isotropic MnBi/α-Fe nanocomposite permanent magnets with different α-Fe content (t vol. %). As t is limited to the range of 5 to 15 vol. %, the magnet exhibits a demagnetization behavior of the single hard phase, indicating ideal exchange coupling effect between the MnBi and α-Fe phases. With 20 vol. % soft phase, a obvious decoupling is observed in the demagnetization curves of the magnet due mainly to the appearance of the soft phase grains whose size are larger than 21 nm in the magnet. Note that the irregular grain shape and the number of finite element could be the reason of the unsmooth in the demagneti-

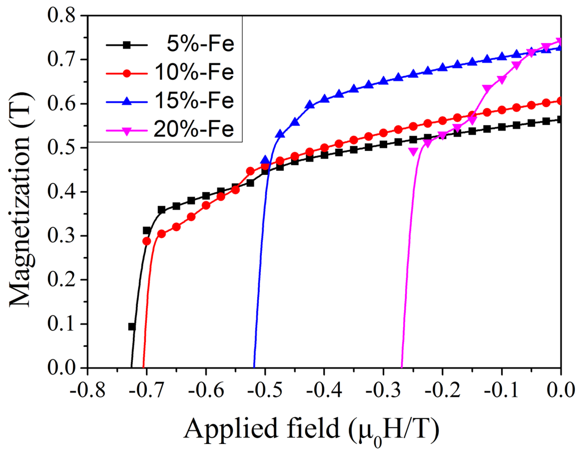

Fig. 3. (Color online) The demagnetization curves of isotropic nanocomposite permanent magnets.

zation curves as the curves for 5-15 vol. % soft phase (as shown in Fig. 3), while it is significant different from the obvious kink resulting from decoupling as shown in the 20 vol. % soft phase curve.

Figure 4 shows the dependencies of saturation magnetization J_s, remanence J_r, remanence ratio ($m_r = J_r/J_s$), coercive force H_{ci}, maximum energy product $(BH)_{max}$ on t.

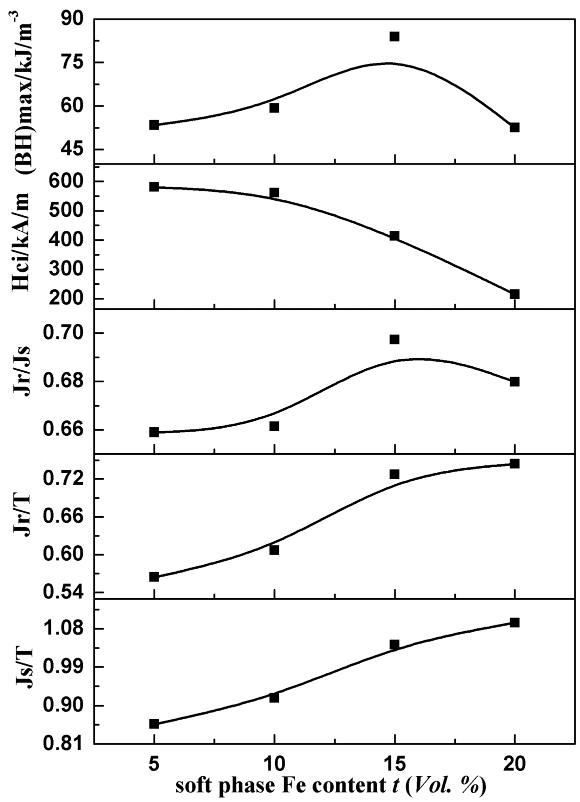

Fig. 4. Magnetic properties of isotropic MnBi/α-Fe nanocomposite permanent magnets as function of the content of α-Fe.

Saturated magnetization J_s and remanence J_r increase with the increase of t, and reach the maximum values, 1.09 T, 0.74 T, respectively, when t = 20 vol. %. Meanwhile the peak value of m_r is 0.697 when t = 15 vol. %, illustrating desirable exchange-coupling effect in this case. The increment of remanence ratio m_r with the increasing of t from 5 to 15 vol. % indicates that α-Fe has benefited to the remanence enhancement effect, then drops with unceasingly increasing of t, because of the presence of big size soft phase grains. Coercive force drops monotonically from 580.9 kA/m to 214.9 kA/m with the increase of t. In the isotropic nanocrystalline magnets, intergranular exchange coupling can enhance the remanence and make coercive force down simultaneously because of the competition between the static magnetic energy and the exchange energy near the grain boundary, leading to the deviation of the magnetic moments from their easy axis in these regions. The maximum energy product reaches the peak, 84 kJ/m^3 (t = 15 vol. %).

3.2. Magnetic Properties of Anisotropic Magnets

Figure 5 shows the anisotropic MnBi/α-Fe nanocomposite magnets' demagnetization curves with single hard phase demagnetization behavior and good squareness, indicating that the alignment of MnBi grains remarkably enhance the exchange coupling effect between the hard and soft phases. However, it is noticeable that with the increase of soft phase content, the squareness of the demagnetization curve is slightly deteriorated due to the weakening of exchange coupling between the hard and soft phases. Figure 6 shows the magnetic properties of anisotropic MnBi/α-Fe nanocomposite magnets as a function of t. In the range of t from 5 to 20 vol. %, m_r approaches 1, and slightly lessens with the increasing of

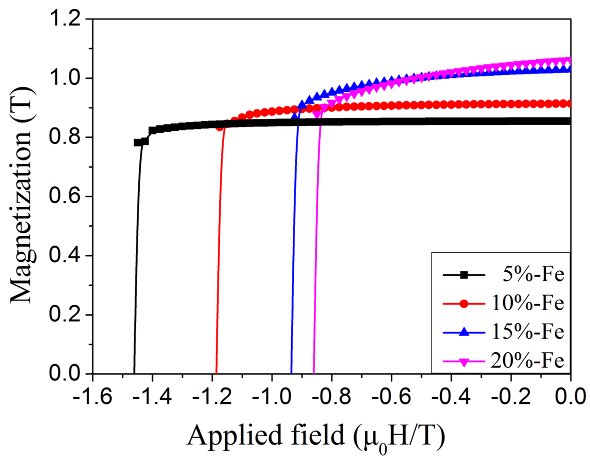

Fig. 5. (Color online) The demagnetization curves of anisotropic nanocomposite permanent magnets.

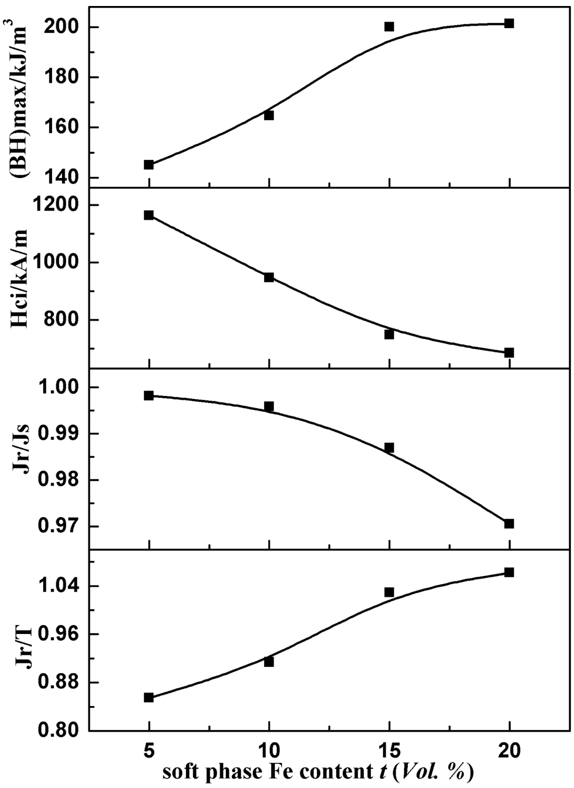

Fig. 6. Magnetic properties of anisotropic MnBi/α-Fe nanocomposite permanent magnets as function of the content of α-Fe.

α-Fe suggesting that parts of magnetic moments deflect from the common easy axis. he deflection occurs mainly in the soft magnetic phase because of the low anisotropy constant in the soft phase. When *t* increases from 5 to 20 vol. %, J_r increases from 0.856 T to 1.06 T, while Hci decreases monotonically from 1163.4 kA/m to 684.4 kA/m. The obtained Hci of 1163.4 kA/m has good agreement with previous experimental Hci of MnBi of 1114 kA/m [15]. In the calculation of MnBi/α-Fe nanocomposite magnets, the anisotropic nanocomposite permanent magnets have higher coercive force than isotropic nanocomposite magnets. This is consistent with report [8] that coercive force increases with the increasing of grain orientation degree, because of strong intergranular exchange coupling effect in nanocrystalline magnets. The maximum energy product $(BH)_{max}$ increases from t = 5 vol. % to t = 15 vol. %, then drops again. The peak value is 200 kJ/m^3. The obtained $(BH)_{max}$ value of 200 kJ/m^3 is lower than the values of 322 kJ/m^3 in the Ref. [5], and the difference of $(BH)_{max}$ comes from the differences between the two calculation models. In detail, the model in the Ref. [5] is an ideal two phase mixture model, in which the hard phase grains scattered regular in the soft phase matrix. On the other hand, the calculation model in this paper are irregular grains of soft and hard magnetic phases that were randomly distributed and the soft phases grains are not in direct contact with each other in the model.

4. Conclusion

The effect of the content of the soft magnetic phase on the magnetic properties was investigated in this paper using micro-magnetic finite element method. Within the range of 5 to 20 vol. % of the α-Fe content, the demagnetization curves of isotropic and anisotropic samples display the feature of single phase magnet, except for the curve of 20 vol. % α-Fe content in the isotropic magnet. The maximum energy product $(BH)_{max}$ reaches maximum value of 84 kJ/m^3, when t is 15 vol. % for isotropic MnBi/α-Fe nanocomposite magnets, while the maximum coercive force H_{ci} is 580.9 kA/m, when t = 5 vol. %. For isotropic MnBi/α-Fe nanocomposite magnets, The maximum value of $(BH)_{max}$ reaches 200 kJ/m^3, when t is 15 vol. %, while the maximum coercive force H_{ci} is 1163.4 kA/m, when t = 5 vol. %. The MnBi/α-Fe nanocomposite magnet has the potential to be a kind of practical magnet.

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