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INTER-GRAIN EXCHANGE INTERACTION FOR SINGLE-PHASE NANOCRYSTALLINE Nd-Fe-B MAGNETS*

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The demagnetization curve as a function of intensity of the inter-grain exchange interaction was calculated for single-phase nanocrystalline Nd-Fe-B magnets by use of the finite-element technique of micromagnetics. Also, the strength of the exchange interaction was estimated as a function of the Nd content x for the nanocrystalline $Nd_xFe_{94-x}B_6$ magnets by comparing the above result with the experimental relation between ${}_{\rm i}H_{\rm c}$ and x for the magnets. We found that the inter-grain exchange interaction decreases with the increase of x, are ≈70% and ≈60% of the inter-grain exchange interaction for x=15.5($\mu_0\,{}_{\rm i}H_{\rm c}$ ≈2.0T) and x=19($\mu_0\,{}_{\rm i}H_{\rm c}$ ≈2.3T), respectively.

Keywords: hysteresis loop, high coercivity materials, rare earth permanent magnet, exchange interaction, micromagnetics

PACC: 7550K, 7550E, 7550W, 7540M

I. INTRODUCTION

A single-phase nanocrystalline Nd-Fe-B permanent magnet is composed of the $Nd_2Fe_{14}B$ grains surrounded by Nd-rich grain boundary phases. The coercivity ${}_{\rm i}H_{\rm c}$ of the magnet increases with the increase of Nd content as a result of the decrease of the inter-grain exchange interaction with the increase of thickness of the Nd-rich paramagnetic grain boundary layer. The inter-grain exchange interaction, which has an important effect on the demagnetization curves, however, has scarcely been studied. Jin *et al.* estimated from the analysis of the temperature dependence of ${}_{\rm i}H_{\rm c}$ that the strength is ≈90% of the inter-grain exchange interaction for the $Nd_{13}Fe_{77}B_{10}$ magnet.[1]

Recently, the experimental relation between ${}_{\rm i}H_{\rm c}$ and Nd content x for the $Nd_xFe_{94-x}B_6$ magnets of grain size 20–30 nm was reported.[2] This work will calculate the demagnetization curve as a function of the strength of the inter-grain exchange interaction for single-phase nanocrystalline Nd-Fe-B magnets or 20 and 30nm grain size by use of the finite-element technique of the micromagnetics. The strength of the inter-grain exchange interaction as a function of the Nd content x of the $Nd_xFe_{94-x}B_6$ magnets will be obtained by comparing the above results with the experimental data of x dependence of ${}_{\rm i}H_{\rm c}$ for the magnets.[2]

II. METHODS AND CALCULATIONS

The demagnetization curve is calculated as follows. The model magnet consists of $N = n\times n\times n$ cubic $Nd_2Fe_{14}B$ grains of size L. The c-axes of the grains are distributed uniformly in the space and are assigned to the grains randomly to simulate the isotropy of the real magnets. Each grain is divided into $m\times m\times m$ cubic elements of single domains. Each element is exchange coupled with the six adjacent elements. The magnet is piled up periodically in the whole space and the periodic boundary conditions of the magnetic properties hold for the magnet.

The energy of the magnet consists of the exchange interaction energy $F_{\rm X}$, the magnetocrystalline anisotropy energy $F_{\rm K}$ and the Zeeman energy $F_{\rm H}$. Since the effect on the curve is small for the magnet,[1] the stray field energy is neglected. The inter-grain exchange interaction between the adjacent elements, say (i,j,k) and $(i+1,j,k)$, is approximated by

$$\begin{aligned} W_{\rm ex} &= \left(\frac{L}{m}\right)^2 \int_i^{l+1} A \sum_{\gamma=x,y,z} (\nabla\alpha_\gamma)^2 {\rm d}x \\ &\approx \left(\frac{L}{m}\right)^2 A \sum_{\gamma=x,y,z} \left[\frac{\alpha_\gamma(i+1,j,k)-\alpha_\gamma(i,j,k)}{L/m}\right]^2 \frac{L}{m} \\ &= \frac{2LA}{m}\left[1-\frac{\boldsymbol{J}_{\rm s}(i,j,k)\cdot\boldsymbol{J}_{\rm s}(i+1,j,k)}{J_{\rm s}^2}\right], \end{aligned} \tag{1}$$

where $\alpha_\gamma(\gamma=x,y,z)$ are the direction cosines of the magnetic polarization vector $\boldsymbol{J}_{\rm s}$. The exchange interaction between the adjacent elements across the grain boundary is also formulated by the same equation but replacing the exchange constant A by $\beta A(0\le\beta\le 1)$. $F_{\rm K}$ and $F_{\rm H}$ are simply the sum of the energies of the

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elements:

$$F_{\rm K}+F_{\rm H}=\left(\frac{L}{m}\right)^3\sum_{i,j,k=1}^{n\times m}[K_1\sin^2\theta_{<100>}(i,j,k)+K_2\sin^4\theta_{<100>}(i,j,k)-\boldsymbol{J}_{\rm s}(i,j,k)\cdot\boldsymbol{H}]. \quad (2)$$

Here $\theta_{<100>}$ is the angle between $\boldsymbol{J}_{\rm s}$ and the c-axis. The values of the magnetic constants for $Nd_2Fe_{14}B$ at room temperature are $\boldsymbol{J}_{\rm s}$=1.63T, A=7.7×10^{-12}J/m, K_1=4.3×10^{6}J/m^3 and K_2=0.65×10^{6}J/m^3.[3] The applied field is decreased from 5T by step $\Delta\mu_0 H$=0.01T, and the magnetic polarization J at each field is obtained from minimization of the energy with respect to the $\boldsymbol{J}_{\rm s}$ directions of the elements $\{(\theta(i),\varphi(i)\}(i=1,2,\cdots,(n\times m)^3)$. The minimization of energy is obtained by using the conjugate gradient method.[4]

Recently we have found that the demagnetization curve, especially $_{\rm i}H_{\rm c}$, calculated by use of the micromagnetics depends strongly on the applied field direction if the number of grains N is not large. The range of the difference and the average value of $_{\rm i}H_{\rm c}$ decreases with the increase of N.[5] The value of $_{\rm i}H_{\rm c}$ for a finite N is larger or at most equal to the limit value $_{\rm i}H_{\rm c}(N=\infty)$ obtained by extrapolation, and so the curve which has the smallest value of $_{\rm i}H_{\rm c}$ among the curves along different field directions for a given N presents the best approximation to the real curve for $N=\infty$.[6]

In this work, the demagnetization curves were preliminarily calculated along several field directions for L=20nm, n=6, m=14 and 16 and β=1; and for L=30nm, n=5, m=18 and β=1. From these field directions, the field direction along which $\mu_0\,{}_{\rm i}H_{\rm c}$ is the smallest was selected for each L. The demagnetization curve as a function of β, then, was calculated along this selected field direction for L=20 and 30nm.

The relation between the inter-grain exchange interaction parameter β and composition x for the $Nd_xFe_{94-x}B_6$ magnet was obtained by comparing the calculated relations between β and $\mu_0\,{}_{\rm i}H_{\rm c}$ and the experimental relation between $\mu_0\,{}_{\rm i}H_{\rm c}$ and x for the compositions of $x\geq$15.5. For the Nd-rich composition region far from the stoichiometric composition x=12, the residual soft magnetic α-Fe phase that strongly disturbs the estimation of the inter-grain exchange interaction should be absent.

Ⅲ. RESULTS AND DISCUSSION

Figure 1 demonstrates $J_{\rm r}/J_{\rm s}$ and $\mu_0\,{}_{\rm i}H_{\rm c}$ calculated along seven different field directions ($\theta_{\rm H}$, $\varphi_{\rm H}$) for m=18 and two directions for m=20, L=30nm, n=5 and β=1. The smallest value of $\mu_0\,{}_{\rm i}H_{\rm c}$ is 1.62T along the field direction of (64, 231) for m=18, and the demagnetization curve as a function of β is calculated along this field direction for L=30nm, n=5, and m=18.

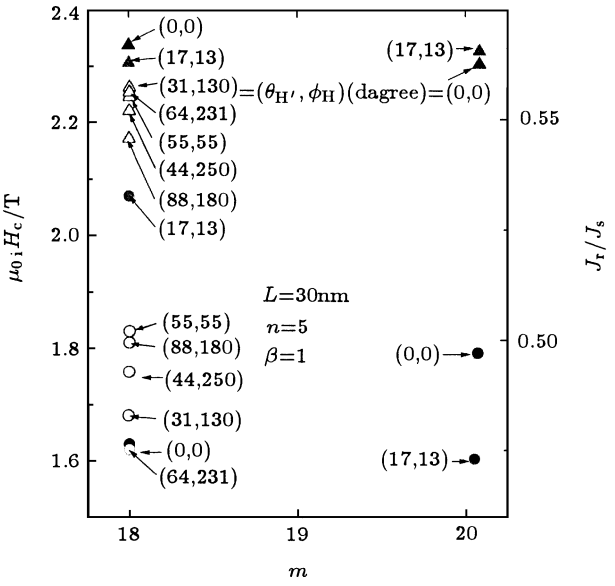


Fig.1. $J_{\rm r}/J_{\rm s}$ (triangle) and $\mu_0\,{}_{\rm i}H_{\rm c}$ (circle) along different field directions for L=30nm, n=5 and β=1.

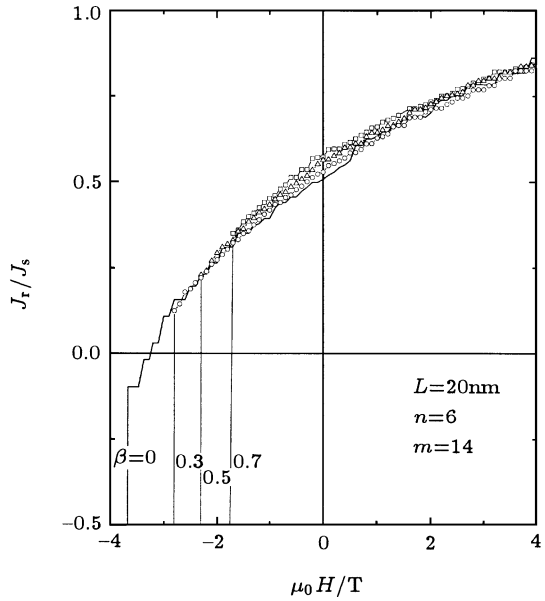


Fig.2. The demagnetization curves for L=20 and β=0(——), 0,3(—◯—), 0.5(—△—) and 0.7(—□—).

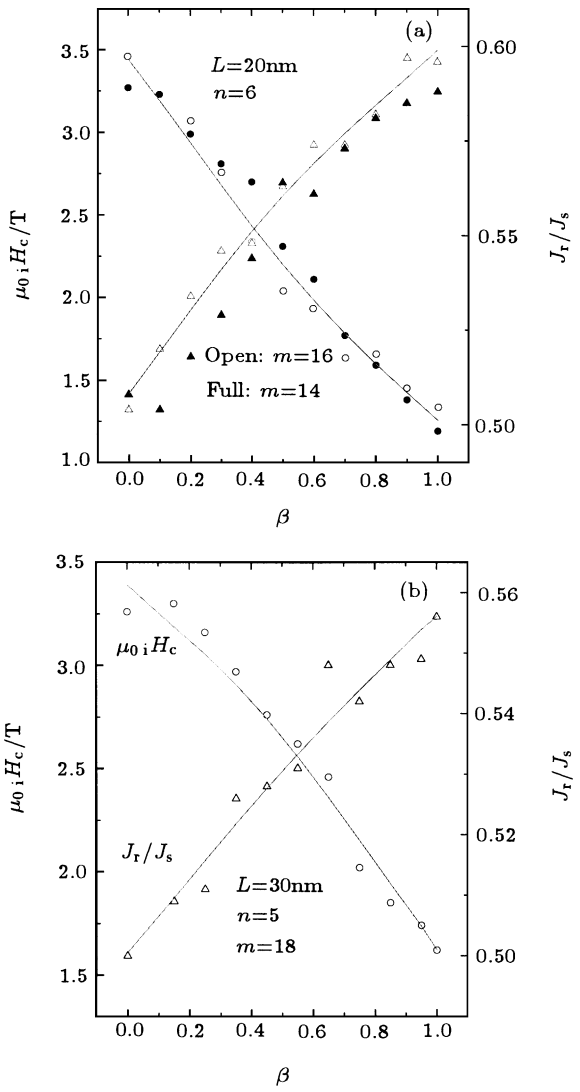


Fig.3. (a) J_r/J_s (triangle) and $\mu_{0\,i}H_c$ (circle) as a function of β for L=20nm; (b) J_r/J_s (triangle) and $\mu_{0\,i}H_c$ (circle) as a function of β for L=30nm.

Figure 2 demonstrates the demagnetization curves calculated for L=20nm, n=6, m=14 and β=0, 0.3, 0.5 and 0.7. It can be seen that β affects mostly $\mu_{0\,i}H_c$. Figures 3(a) and 3(b) show J_r/J_s and $\mu_{0\,i}H_c$ as functions of β for L=20 and 30nm, respectively. With the decrease of β from 1 to 0, J_r/J_s decreases from 0.59 to 0.50 and $\mu_{0\,i}H_c$ increases from 1.2 to 3.4T for L=20nm, and J_r/J_s decreases from 0.55 to 0.50 and $\mu_{0\,i}H_c$ increases from 1.6 to 3.4 T for L=30nm.

Figure 4 shows the x dependence of β (for L=30 and 20nm) and $\mu_{0\,i}H_c$. Since the grain size of the $Nd_xFe_{94-x}B_6$ magnet is between 20 and 30nm,[2] β as a function of x in the magnet of experiment[2] should be located between the two curves obtained for L=20 and 30nm. β decreases with the increase of x, and is 0.7±0.1 for x=15.5($\mu_{0\,i}H_c$ ≈2.0T) and 0.6± 0.1 for x=19($\mu_{0\,i}H_c$ ≈2.3T).

The results show that the inter-grain exchange interaction remains strong and cannot be neglected for high coercivity Nd-rich magnet.

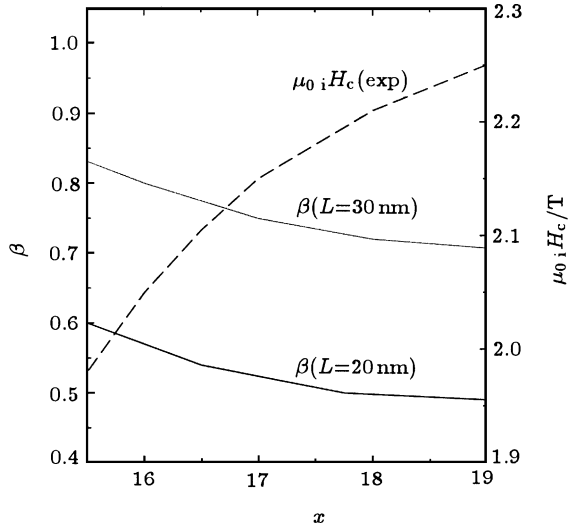


Fig.4. β and $\mu_{0\,i}H_c$ as functions of x for the magnets of $Nd_xFe_{94-x}B_6$.

References

[1] Jin H M, Kim Y B and Wang X F 1998 *J. Phys.: Condens. Matter* **10** 7243

[2] Ahmad I, Davies H A and Buckley R A 1996 *J. Magn. Magn. Mater.* **157/158** 31

[3] Fischer R, Schrefle T, Kronmuller H and Fidler J 1996 *J. Magn. Magn. Mater.* **153** 35

[4] Grill P, Murray W and Wright M H 1981 *Practical Optimization* (London: Academic)

[5] Jin H M, Zhao S F and Wang X F 2000 *J. Mater. Sci. Technol.* **16** 107

[6] Jin H M, Wang X F, Zhao S F and Yan Y 2001 *Chin. Phys.* **10** accepted for publication