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Effects of grain boundary configuration and characteristics on the demagnetization process and coercivity of anisotropic NdFeB magnets

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ABSTRACT

A systematic investigation on the effects of grain boundary configuration and characteristics on the demagnetization process and magnetic properties of NdFeB magnets is carried out by micromagnetic simulation based on a periodic anisotropic model. The results indicate that, when the grain boundary phase is perpendicular to the easy axis, the demagnetization field is along the positive Z axis and the magnetic moments rotate difficultly due to the dipolar coupling. When the grain boundary phase is parallel to the easy axis, the demagnetization field is along the negative Z axis and the magnetic moments rotate easily. The best hard magnetic properties can be obtained by reducing the thickness and saturation magnetization of grain boundary phase distributed parallel to the easy axis and reducing the exchange stiffness of grain boundary phase perpendicular to the easy axis.

1. Introduction

Microstructure optimization is a key impact for permanent magnetic materials in order to improve their magnetic properties. Particularly, the intergranular phases play an important role in determining the magnetic properties of the NdFeB magnets, especially for the coercivity [1]. Grain boundary diffusion (GBD) has been considered as an effective way to optimize microstructure, mainly the structure and distribution of the intergranular phases [2,3]. It is well known that increasing the thickness of intergranular RE-rich phases is beneficial to enhance coercivity due to their decoupling effect [4].

Regarding the commercial anisotropic NdFeB magnets, the intergranular phases (mainly thin layers) can be divided into two types according to their orientation relationship with the easy axis, i.e. grain boundary (GB) phases parallel to the easy axis and GB phase perpendicular to the easy axis. Recently, Sasaki et al. [5,6] investigated the microstructure of the anisotropic Nd-Fe-B sintered magnets and revealed that the GB phases perpendicular to the easy axis was mostly crystallized with a high Nd concentration, whereas that nearly parallel to the easy axis had the amorphous structure with a high Fe concentration. The former is regarded as a paramagnetic phase and the later is considered to be soft-ferromagnetic [7]. The magnetic characteristics of those GB phases have significant effects on the magnetic properties, which are difficult to be investigated by experiments. Hence, micromagnetic modeling may be a good way.

On the other hand, the thickness of GB phase is another important factor governing the extrinsic magnetic properties of NdFeB magnets. In the hot deformed anisotropic nanocrystalline magnets, the thickness of GB phase is related to the relative position of the easy axis [7]. The thickness of GB phases perpendicular to the easy axis and GB phases parallel to the easy axis may have different effects on magnetic properties. Unfortunately, the effects are still unclear. To better understand the effects of GB phase thickness, the simulation is also a good approach.

Hence, in this work, the effects of the thickness, distribution, and magnetic parameters of the GB phase on the demagnetization process and magnetic properties of NdFeB magnets have been studied by micromagnetic simulation, which has proved to be effective in resolving the magnetic physical problems regarding the microstructure which cannot be fully realized in real case [8].

2. Simulation method

Micromagnetics is a phenomenological theory that explains mesoscopic magnetic phenomena based on the energy minimization and classical field theories, which utilize the continuously differentiable magnetization vectors as thermodynamic coordinate.

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The basic equations in micromagnetism are the energy minimization equation and Landau-Lifshitz-Gilbert (LLG) equation [9], showing as follows,

$$E_t = E_{ex} + E_a + E_d + E_H = f(\boldsymbol{M}) \quad (1)$$

$$\frac{\partial \boldsymbol{M}}{\partial t} = \alpha \boldsymbol{M} \times H_{eff} + \beta \boldsymbol{M} \times (\boldsymbol{M} \times H_{eff}) \quad (2)$$

where $\boldsymbol{M}$ is the magnetization vector. E_t, E_{ex}, E_a, E_d, E_H in Eq. (1) are the total energy, exchange coupling energy, anisotropy energy, stray energy, and Zeeman energy, respectively. Eq. (2) is also the rotation equation of the magnetization vector under the effective field. The effective field

$$H_{eff} = -\frac{1}{M_S}\frac{\partial E_t}{\partial \boldsymbol{M}} \quad (3)$$

is the equivalent field of the total energy influence on the magnetization vector. α and β are the constant coefficients for precession part and damping part, respectively.

To investigate the effects of grain boundary phase on the demagnetization process and magnetic properties of the anisotropic NdFeB magnets, the simulation model is set up using OOMMF software [10]. Driver "Oxs_MinDriver" and solver "Oxs_CGEvolve" are used in this simulation, and the simulation parameters are defined in these parts. One of the most important parameters is the convergence criteria, stopping_mxHxm, and it is set as 0.1 in this work. The applied field changes from 7000 kA/m to −7000 kA/m with 10 kA/m for one step, which is similar to experimental test parameters. The maximum of iterations for one stage "Stage_iteration_limit" is set as 10,000, which limits the iterations in every stage less than 1000.

As shown in Fig. 1, the easy axis of anisotropic nanocrystalline NdFeB grains and period direction are both along with the Z axis. The grey cuboids (mainly 100 nm ∗ 100 nm ∗ 100 nm) are $Nd_2Fe_{14}B$ grains. The red cube (50 nm ∗ 50 nm ∗ 50 nm) is the Nd-rich phase, representing the nonmagnetic particles or defects. The nonmagnetic particle is a typical structure in NdFeB magnet [11], its top surface and bottom surface are easy to be the nucleation sites. The direct contact between the grain boundary and the nonmagnetic particle is also representative in NdFeB magnets [12]. The green and yellow thin layers are the GB phases parallel to the easy axis (XYGB, for short) and perpendicular to the easy axis (ZGB, for short), respectively. The mesh size is 2.5 nm ∗ 2.5 nm ∗ 2.5 nm. The model used in this work is a periodic model which neglects the macro-demagnetization field. If the periodic boundary condition was not assumed in our modeling, the shape and macro-demagnetizing field of the model would influence the nucleation and demagnetization processes significantly. Hence, the nucleation would easily occur near the top and bottom surfaces, where macro-demagnetizing field was large [13]. While the effects of the microstructure and grain boundary configurations would be neglected. All the simulation results presented in this work are repeatable.

The room temperature magnetic parameters of $Nd_2Fe_{14}B$ phase taken from Ref. [14] by Schrefl et al. are listed in Table 1. The parameters of nonmagnetic particle are all set to zero. The magnetocrystalline anisotropy constant K_1 is set to zero in all GB phases [8,15]. Reduction factors are introduced to set the magnetic parameters of the GB phases proportional to those of $Nd_2Fe_{14}B$ grains. P_{xy} is the reduction factor of the saturation magnetization J_s in XYGB, P_z is the reduction factor of the saturation magnetization J_s in ZGB, Q_{xy} is the reduction factor of the exchange stiffness A in XYGB, and Q_z is the reduction factor of the exchange stiffness A in ZGB.

3. Results and discussion

3.1. Effects of grain boundary phase thickness

To investigate the effects of the GB phase thickness, the values of P_{xy}, Q_{xy}, P_z and Q_z are all set to 0.6. Fig. 2(a) and (b) shows the demagnetization curves and coercivities of the samples changing with GB thicknesses (2.5 nm, 5.0 nm and 10 nm). The GB structures are simplified as XYGB x nm–ZGB y nm. For example, XYGB 2.5 nm-ZGB 5 nm indicates the thicknesses of the grain boundary phases parallel and perpendicular to Z axis are 2.5 nm and 5 nm respectively. The calculated coercivities are much higher than the experimental values (1050 kA/m [16], 820 kA/m [17]) due to the neglected macroscopic demagnetization field [18] and more simplified model. The results indicate that the ferromagnetic GB phase is not beneficial for the magnetic properties and the coercivity decreases with the increasing thickness of XYGB (and ZGB), which are in a good agreement with the experimental results [19,20]. It is interesting that the XYGB thickness has stronger effect on the coercivity than the ZGB thickness does. The coercivity reduces more rapidly with the increasing XYGB thickness (Fig. 2(b)). The reason may be due to that the distribution of demagnetization field is more sensitive to the change of XYGB thickness, and thus the nucleation field is also sensitive to the variation of XYGB thickness.

Three different kinds of demagnetization curves can be observed in Fig. 2(a), including standard square loops, square loops with a slow slope, and square loops with a steep slope, which corresponded to XYGB 2.5 nm-ZGB 2.5 nm, XYGB 2.5 nm-ZGB 10 nm, and XYGB 10 nm-ZGB 2.5 nm samples respectively. The magnetic vector distributions and the magnetization configurations during

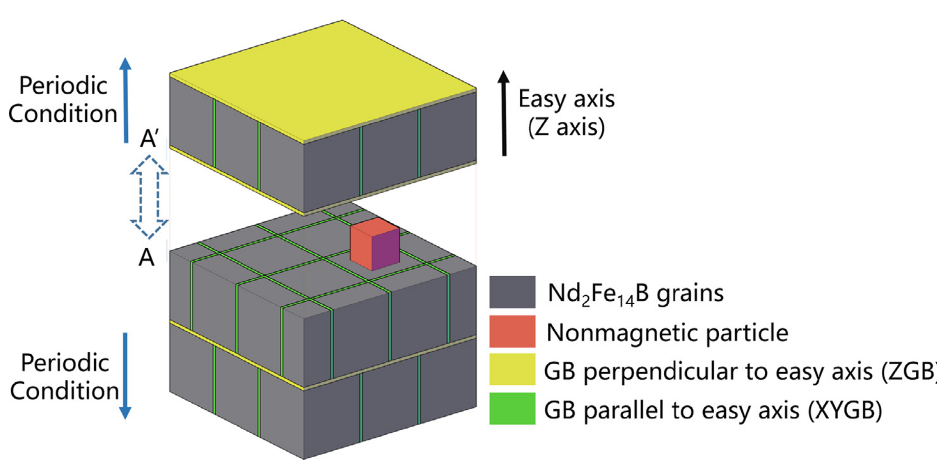

Fig. 1. The simulation model.