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Micromagnetic finite element simulation of nanocrystalline α-Fe/$Nd_2Fe_{14}B$/Fe_3B magnets

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ABSTRACT

Nanocomposite $Nd_2Fe_{14}B$ permanent magnets with Fe_3B and α-Fe as the soft phase have been simulated using micromagnetic modelling. This paper reviews extensively the results from the simulation point of view. The magnetization configuration along the hysteresis loop is discussed in details. It was clear that the grain size and phase distribution play important roles in determining the magnetic properties. By changing the size of the grain and the volume fraction of the hard and soft phase, the magnetic properties change and the relationship between microstructure and properties is investigated. The remanence, J_r increases with decreasing of grain size, but oppositely for coercivity, H_c. The highest J_r, 1.46 T was obtained with a grain size 10 nm, and volume fraction of α-Fe, 40%. Whereas, the highest H_c with combination $Nd_2Fe_{14}B$ 80% and 20% Fe_3B, 947 kA/m. On the other hand, if $Nd_2Fe_{14}B$ alone, the H_c able to reach up to 1000 kA/m. From this study, micromagnetic modelling contributes to a better understanding how microstructure and phase distribution influences the magnetic properties.

1. Introduction

Micromagnetic modelling, using finite-element calculations give a quantitative description of the reciprocal relationship between the microstructure [1,2] and magnetic properties such as hysteresis parameters [3–7]. The micromagnetism characterises the magnetization processes on a significant length scale which is large enough to replace the atomic spin and small enough to resolve the transition between magnetic domains [6,8]. As a result, it contributes to the understanding of the basic mechanism that determine the magnetic properties and their correlation with microstructural features [1] such as grain size particle shape and intergranular phases [9].

There has been lot of research involving micromagnetic simulations particularly on nanocomposite permanent magnets [7,10–13] over the past 20 years [14]. Kneller [15] was the individual who studied in detail the 1-D modelling of the relationship between the soft and hard phases in nanocomposite permanent magnets. Micromagnetic modelling contributes to achieving a greater understanding of the optimisation of the microstructural and magnetic properties [1].

Owing to their advantages such as high remanence and relatively low cost, these materials are of particular interest for detailed investigation. These magnets are a combination of magnetically hard and soft phases (α-Fe or Fe_3B) without any intergranular phases as described by several researcher [1,4,16]. The grain structure shown in the model consists of randomly distributed polyhedral grains. In numerical simulations, most of the important parameters to be considered are the grain sizes, the volume fraction of the phases, the magnetisation distribution, the grain numbers and the grain shapes.

In general, isotropic permanent magnets with a remanence ratio (J_s is a saturation polarisation), $J_r/J_s > 0.5$ are claimed as remanence enhanced materials [17–19]. Yet, the theoretical limit for randomly oriented grains depends on the crystal symmetry, the crystallographic orientation of the easy axis, the volume fraction, and the saturation polarisation for both, magnetically hard and soft phases [3,15]. Hysteresis loops for randomly oriented grains having uniaxial anisotropy were calculated on the basis of 512 grains which interacted by exchange coupling at the grain boundaries. The aim of the numerical simulation is to gain better understanding of magnetization reversal, together with the spin configuration along the hysteresis loop. In addition, this work reveals how microstructure and phase distribution contributes to the magnetic properties.

2. Method

The micromagnetic simulation technique is principally based on work done by Schrefl [7,10–13]. This method is developed from

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the direct minimization of the total magnetic Gibbs free energy and the time integration of the Gilbert equation of motion. The total magnetic Gibbs free energy which [9,20] is the sum of the exchange energy, the magnetostatic energy, the magnetocrystalline anisotropy energy and the Zeeman energy [21]. The minimisation of the total magnetic Gibbs free energy [1,4,6]:

$$E_t = E_{\text{exchange}} + E_{\text{anisotropy}} + E_{\text{magnetostatic}} + E_{\text{zeeman}}$$

$$E_t = \int \left[A \sum_{i=1}^{3} (\nabla \beta_i)^2 + f_k(J) - \frac{1}{2} J \times H_d - J \times H_{ext} \right] dV \quad (1)$$

with respect to the magnetic polarisation $J=\beta J_s$, subject to the constraint $|J| = J_s$. A is the exchange constant, H_d is the demagnetisation field, H_{ext} is the external field, and f_k is the energy density associated with magnetocrystalline anisotropy.

The theoretical limit for remanence and coercive field were determined for nanocrystalline composite hard magnets with various ratios between the $Nd_2Fe_{14}B$ ($J_s=1.61$ T, $K_1=4.2$ MJ/m^3 [22], $A=7.7$ pJ/m [23] hard phase, and the α-Fe ($J_s=2.15$ T, $K_1=0.046$ MJ/m^3, $K_2=0.015$ MJ/m^3, $A=25$ pJ/m) and Fe_3B ($J_s=1.62$ T, $K_1=-0.32$ MJ/m^3, $A=12.5$ pJ/m) soft phases [24].

The model has been developed close as possible to the real magnet, but at the same time attempting has been made to make it simple and uncomplicated. Thus, in order to develop the model, few assumptions have been made. The model is established as a cubic shape as compared to the magnetic ribbon in the real magnet (Fig. 1). It has 512 grains with irregular shape where in real magnet the grain has uneven in shape. There are 3 different phases contribute to generate the simulation which are $Nd_2Fe_{14}B$, Fe_3B and α-Fe. Furthermore, the grains are directly contacting and randomly distributed with all phases have the same grain size ranging from 10 nm to 30 nm.

3. Results and discussion

3.1. Magnetization reversal of isotropic nanocomposite $Nd_2Fe_{14}B$/Fe_3B/α-Fe permanent magnets

The magnetization distribution for a nanocomposite magnets consisting of 60% of hard phase $Nd_2Fe_{14}B$, 20% of Fe_3B and 20% of α-Fe at different states has been shown in Fig. 2. The images of the cross section in the middle of the cubical model are similar to what have been done by Schrefl et al. [5]. The directions of the easy axes of $Nd_2Fe_{14}B$ grains are isotropically distributed [25]. Also the orientations of α-Fe grains with cubic anisotropy are randomly diffused. An applied field of up to 4T is applied along the easy axis.

In the initial state (Fig. 2a), the grains are irregularly distributed and the magnetization configuration in all phases behave differently. The easy axes of some hard phases are oriented towards the applied field which contribute to the non-zero magnetic polarisation, J. As the field is gradually increased (Fig. 2b), the spins (Fe_3B) of the soft phase in circle 1 are immediately rotated following the z direction and saturated (circle 3). The completed saturations have been seen in α-Fe grains. Since both of the soft phases have very low magnetocrystalline anisotropy, they are more easily aligned parallel to the field than the hard phase. Due to the high magnetocrystalline anisotropy of the hard phase, it is difficult to rotate the magnetisation as can be seen in circles 2 and 4.

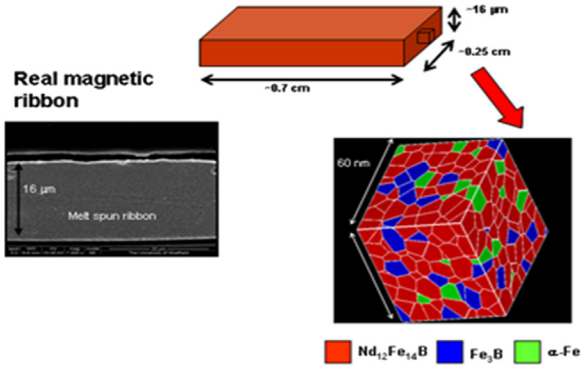

Fig. 1. Development of finite element model based on melt spun magnetic ribbon.

At a high external field of 4 T, the magnetization of all grains points upward in the z direction (Fig. 2c). Thus after a large field is applied the magnetisation of the hard phases is completely rotated as in circle 5. As the field is gradually reduced to zero, (Fig. 2d) the magnetisation of the hard magnetic grains rotates towards the direction of the local easy axis. At the same time, the magnetization of the soft magnetic grains remains parallel to the field direction. Indeed, the soft phase, especially α-Fe gives the high remanence to the nanocomposite permanent magnets.

For an applied field, as low as 0.4 T (Fig. 2e), the magnetization of the soft magnetic grains is gradually rotated opposite to the direction of the applied field. The circle 6 and 8 shows the different orientations of the soft phase. If the field is removed, the magnetization of the soft grains will rotate back to its original direction which is the so called exchange-spring effect. However, when the reverse field is high enough the hard grains start to rotate, thus leading to irreversible magnetization reversal [15].

Furthermore, when the reverse field is increased to 0.75 T (Fig. 2f), all of the soft phases are already saturated in the negative direction as shown in circle 10. There are few areas where the spin for the hard grains are pointing opposite to the z. In spite of this, several hard phases need a higher field to rotate, as in circles 7 and 9. By increasing the applied field to 2.4 T (Fig. 2g), the grain in circle 11 is saturated. In order to make sure that all grains are completely saturated in reverse direction, the reversed field again needs to rise up to 4 T (Fig. 2h). In this state, an apparent rotation of hard grains is clearly demonstrated in circles 12 and 13.

4. Remanence enhancement

Fischer et al. [7] provided guidelines for optimising the grain structure to enhance the remanence of isotropic nanocomposite magnets. The average grain size for soft and hard grains must be <20 nm. In addition, the grains are arranged to be in direct contact and have no intergranular phase. In this section, contribution of soft phase, α-Fe and Fe_3B, has been studied in order to enhance the remanence as reported elsewhere [11,13,25], thus, the fixed ratio of soft and hard phase have been made to 20:80 and 40:60.

The grain-size dependence of the remanence of isotropic nanocomposite permanent magnets consisting of 20% and 40% of α-Fe and F_3B are shown in Fig. 3. As elsewhere [11,13,25], remanence always decreases with increasing grain size. The highest remanence, 1.46 T was obtained with a grain size of 10 nm and volume with 40% of α-Fe. For a grain size of 30 nm for the same fraction of α-Fe the remanence is 1.33 T. For a lower volume fraction of α-Fe, of 20% volume, the curve shows a maximum remanence of 1.28 T with a grain size of 10 nm. The higher the volume fraction of the soft phase, the higher the remanence, but it is the opposite for coercivity as established by Coehoorn [26] and Davies [17]. These simulation results presented the agreement with those reported previously. Theoretically, when the grain size increases, the remanence rapidly decreases [13,27,28]. This can be explained by the exchange coupling between hard and soft grains which become weaker as compared to the other micromagnetic energy terms when the grain size increases.