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Effect of grain size and distribution on the anisotropy and coercivity of nanocrystalline $Nd_2Fe_{14}B$ magnets

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Abstract

The effect of grain size and distribution on the anisotropy and coercivity of nanocrystalline $Nd_2Fe_{14}B$ magnets has been studied by adopting a Gaussian distribution model of grain sizes. The results show that the effective anisotropy K_{eff} and coercivity H_c decrease with reducing average grain size $\bar{D}$, and the decrease is more rapid when $\bar{D} < 15$ nm. The nonideal distribution of grain size results in a further decrease of K_{eff} and H_c. The grain size distribution has greater effect on K_{eff} when $\bar{D} > 15$ nm. Taking values of the microstructure constant $P_c = 0.9$ and distribution coefficient $\sigma = 0.5$, the variation of H_c with $\bar{D}$ is consistent with published experiment results. The decrease of H_c is mainly attributed to the decrease of K_{eff}. In order to obtain high effective anisotropy and coercivity in nanocrystalline $Nd_2Fe_{14}B$ magnets, $\bar{D}$ should be larger than 15 nm and the grain size distribution should be as centralized as possible.

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1. Introduction

Grain size of magnetic materials is an important structural factor critically influencing the magnetic properties. Some investigations about the effect of nanometer grain size on magnetic properties of magnets have been done. Herzer [1] pointed out that the anisotropy and coercivity of Fe-based nanometer soft magnetic material decreases rapidly with reducing grain size. The experimental study on the nanocrystalline NdFeB material given by Manaf et al. [2] showed that when the grain size is less than 40 nm, remanence increases obviously while coercivity decreases rapidly. Gao et al. [3] expatiated that the effective anisotropy decreases with the reduction of grain size in nanocomposite permanent magnets, and when the grain sizes reduce to 4–5 nm, K_{eff} decreases to $\frac{1}{3}$–$\frac{1}{4}$ of the ordinary value of K. Feng et al. [4] reported when the grain sizes of the soft and hard phases are identical and the volume fraction of the soft phase is given, the coercivity decreases with the reduction of grain size. The results of Han et al. [5] showed that the exchange-coupling interaction between grains causes a decrease of the effective anisotropy with decreasing grain size. The results mentioned above are obtained at the condition of uniform grain sizes. In general, the grain sizes are nonuniform and have certain distributions [6]. In this paper, we studied the effect of grain size and distribution on the anisotropy and coercivity of nanometer magnets by adopting the cube model of grain structure [7] and the Gaussian distribution model of grain size.

2. Effective anisotropy and coercivity of nanometer hard magnets

2.1. Effective anisotropy of nanometer hard magnets with uniform grain size

For the uniform grain size the results of Ref. [7] showed: when the grain size D is larger than the exchange-coupling length L_{ex}, there exist partial exchange-coupling

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interactions between grains (inner part without exchange-coupling interaction (uncoupled) and interfacial part with exchange-coupling interaction (coupled)). The effective anisotropy can be expressed as follows:

$$\langle K\rangle = K_1 v^{\mathrm{int}} + \langle K_1^{\mathrm{lay}}\rangle v^{\mathrm{lay}}, \tag{1}$$

where v^{int} and v^{lay} are the volume fraction of uncoupled and coupled part of the grain, respectively. $\langle K_1^{\mathrm{lay}}\rangle$ is the average anisotropy constant of coupled part. In uncoupled part of grains, the anisotropy constant is the common anisotropy constant of material K_1. The anisotropy constant in the coupled part, $K_1^{\mathrm{lay}}(r)$, is supposed to vary in a similar manner of the random anisotropy expressed by Herzer [1] and can be described as follows:

$$K_1^{\mathrm{lay}}(r) = K_1(2r/L_{\mathrm{ex}})^{3/2} \tag{2}$$

and $\langle K_1^{\mathrm{lay}}\rangle$ can be obtained by the integral

$$\langle K_1^{\mathrm{lay}}\rangle = (V^{\mathrm{lay}})^{-1}\int K_1^{\mathrm{lay}}(r)\,\mathrm{d}v, \tag{3}$$

where V^{lay} is the volume of coupled part. Assuming that the grains are regular cubes with edge length D as illustrated in Fig. 1, considering the coupling situation of 6 surface layer is parity, V^{lay} and $\langle K_1^{\mathrm{lay}}(r)\rangle$ can be expressed as follows:

$$V^{\mathrm{lay}} = 6\int_0^{L_{\mathrm{ex}}/2}(D-2r)^2\,\mathrm{d}r = D^3 - (D-L_{\mathrm{ex}})^3, \tag{4}$$

$$\langle K_1^{\mathrm{lay}}\rangle = \frac{6}{V^{\mathrm{lay}}}\int_0^{L_{\mathrm{ex}}/2} K_1(2r/L_{\mathrm{ex}})^{3/2}(D-2r)^2\,\mathrm{d}r. \tag{5}$$

2.2. *Effect of the grain size distribution on effective anisotropy*

Considering the grain size distribution $f(D)$, the effective anisotropy K_{eff} can be expressed as follows:

$$K_{\mathrm{eff}} = \frac{\int_a^b \langle K\rangle f(D)\,\mathrm{d}D}{\int_a^b f(D)\,\mathrm{d}D}, \tag{6}$$

where a and b are the minimum and maximum of grain size. We adopt the Gaussian distribution model to describe the grain size distribution

$$f(D) = \frac{1}{\sigma'\sqrt{2\pi}}\exp\left\{-\frac{(D-\bar{D})^2}{2\sigma'^2}\right\}, \tag{7}$$

where $\bar{D}$ is the average grain size and σ' is the distribution coefficient describing the distribution centralized degree. The smaller the σ' is, the more centralized the distribution is. When $\sigma' = 0$, the grain size is uniform, which is called ideal distribution. Eq. (7) can be rewritten as

$$f(D) = \frac{1}{\bar{D}\sigma\sqrt{2\pi}}\exp\left\{-\frac{((D/\bar{D})-1)^2}{2\sigma^2}\right\}, \tag{8}$$

where $\sigma = \sigma'/\bar{D}$. Fig. 2 expresses the Gaussian distributions of normalized grain size $(D/\bar{D})$ for different σ.

2.3. *Coercivity of nanometer hard magnets*

Herzer [1] described the coercivity of nanometer permanent magnets as

$$H_{\mathrm{c}} = p_{\mathrm{c}}\frac{\langle K\rangle}{J_{\mathrm{s}}}, \tag{9}$$

where p_{c} is a dimensionless factor which depends on the microstructure and particular magnetization process of

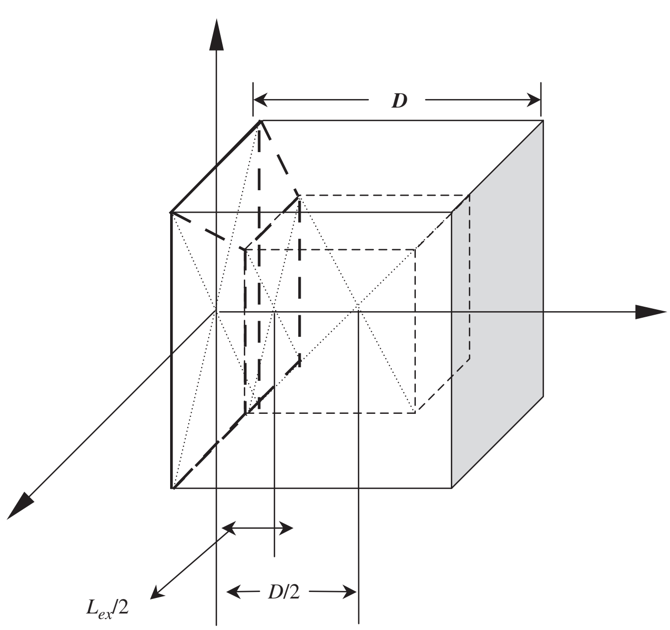

Fig. 1. Cube model of grain structure.

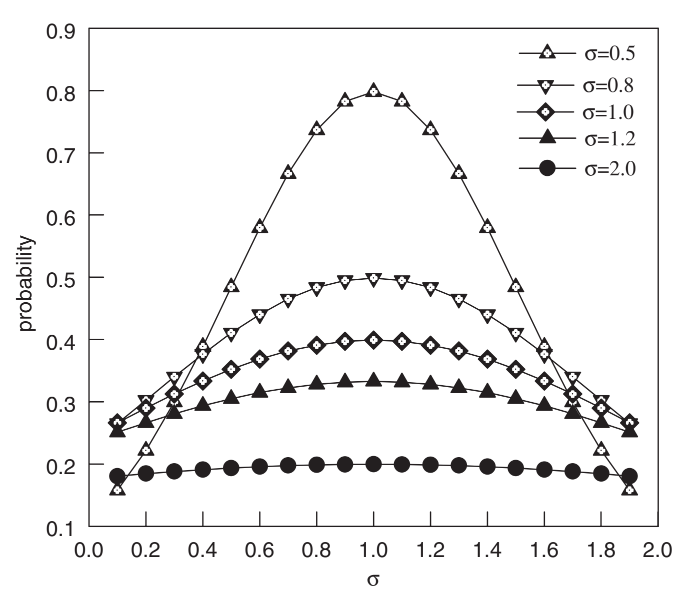

Fig. 2. Gaussian distributions of normalized grain size $(D/\bar{D})$ for different σ.