Remanence enhancement of single-phased isotropic nanostructured permanent magnets

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Abstract

Based on a simple micromagnet model, we show that an analytical expression for reduced remanence in single-phased and single-domain isotropic nanostructured permanent magnetic materials can be written as $M_r/M_s = 0.5 + 1.8\Delta_0/L$, where $M_r, M_s, \Delta_0$, and $L$ are the remanence, saturation magnetization, exchange length and the average grain size, respectively. This formula reveals that our calculated remanence is larger than the predictions of the Stoner–Wohlfarth model for all particle sizes, and that remanence enhancement increases with decreasing grain size. Application of the relation to melt-spun Nd–Fe–B magnets shows good agreement with available experimental and numerical data. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

The performance of a permanent magnetic material is largely dependent on the maximum magnetic energy product $(BH)_{\text{max}}$, the remanence $M_r$ and the coercivity $H_c$. Because of their large remanence and coercivity, rare-earth iron and rare-earth cobalt magnetic materials have attracted much attention in recent years. The coercivity of a material is a measure of the magnet's resistance against demagnetizing field and can be improved by various ways, including the hardening process.

Remanence determines the strength of the material. According to the Stoner–Wohlfarth (SW) model, for an assembly of non-interacting and randomly oriented grains, the ratio of the remanent magnetization $M_r$ to the saturation magnetization $M_s$ is $0.5$ [1]. However, nanocrystalline isotropic permanent magnets show in general an enhanced remanence in which the ratio is larger than 0.5 [2]. Remanence enhancement of a permanent magnetic material can be achieved in two ways, firstly, by adding soft-phased material to the hard-phased bulk, and secondly, by making the particle small.
compared to the thickness of the domain wall of the material.

There have been many experimental and theoretical studies on remanence enhancement in two-phased magnetic materials [2–10]. Remanence enhancement in single-phased magnetic materials has also been studied [2,3,7,11–14]. Recent rapid quenching techniques, such as melt-spinning [5–7] or mechanically alloying [8–10], can produce single-domain rare-earth iron or rare-earth cobalt magnetic grains of nanosstructured scale, which display randomly oriented easy axis distributions. Studies have shown that large remanence enhancement can be achieved with smaller particle size, both in single-phased and two-phased materials. Numerical calculations, such as Monte-Carlo or finite-element approaches, have further established that the exchange interactions in the grain boundaries are responsible for remanence enhancement of small particles [2,3,11–14]. The exchange interactions cause the magnetization to deviate from the easy axis directions, resulting in remanence enhancement. However, because of the mathematical difficulties involved, detailed analytical work of remanence enhancement of nanostructured permanent magnetic materials taking into account random easy axis distribution is still lacking. Previous analytical works deal exclusively with special easy axis direction (parallel to the applied field direction [15,16]). In the present work, we derive an analytical formula for remanence enhancement based on a simple micromagnetic model, taking into account only anisotropy and exchange energies. This approach allows us to calculate remanence enhancement for smaller grains that exhibit random easy axis distributions. The exchange energy, neglected in the SW model [1], is used to model the intergrain interactions within a collection of interacting magnetic grains.

2. The analytical model

The magnetic properties, i.e., remanence, coercivity and the maximum energy product of a ferromagnet are usually presented using an $M-H$ plot or hysteresis loop. The macroscopic magnetization $M$ is obtained by averaging the spontaneous magnetization $M_s(r)$ over the entire volume. While the magnitude of the spontaneous magnetization is a constant $M_s$, the orientation of the magnetization is determined by the applied magnetic field $H_{app}$ and the local easy axis direction. Theoretically, these orientations can be determined by minimizing the total Gibbs free energy $G$ so as to yield a stable equilibrium state for a magnetic structure consisting of many nanostructured magnetic grains. The total Gibbs free energy of the system is given by

$$G = \iiint \Phi_i \, dv,$$

where $\Phi_i$, the total magnetic free energy density, can be written [17] as

$$\Phi_i = \Phi_e + \Phi_K + \Phi_S + \Phi_H.$$

Here $\Phi_e$ is the exchange energy density, $\Phi_K$ is the magnetocrystalline anisotropy energy density for a uniaxial system, $\Phi_S$ is the stray field energy density and $\Phi_H$ is the magnetostatic energy density. The exchange energy, given by the Heisenberg Hamiltonian, favors parallel alignment of the magnetic moments in a ferromagnetic material with positive exchange interaction. Using spherical coordinates $\theta(r)$ and $\psi(r)$ (cf. Fig. 1) to indicate the orientation of the spontaneous magnetization $M_s(r)$ at $r$, the exchange energy density $\Phi_e$ can be written as

$$\Phi_e = A[(\nabla \theta(r))^2 + (\nabla \psi(r))^2 \sin^2 \theta(r)],$$

where $A$ is the isotropic exchange constant. The magnetocrystalline anisotropy energy describes the tendency for the magnetization to align along certain preferable crystalline direction, i.e., the easy axis direction. Ignoring higher-order terms, the magnetocrystalline anisotropy energy can be written as

$$\Phi_K = K \sin^2 \phi(r),$$

where $K$ is a constant and $\phi(r)$ (see Fig. 1) is the angle between the spontaneous magnetization at $r$ and the direction of the easy axis. The stray field energy density is given by

$$\Phi_s = -\frac{1}{2} \mu_0 H_0(r) \cdot M_s(r),$$
where \( \mathbf{H}_s(r) \) is the stray field. The stray field energy accounts for the long-range magnetostatic interaction and is important in determining the magnetization distribution. However, the remanence enhancement is mainly attributed to the inter-grain exchange interactions \([2,13,14]\), which play a dominant role compared to the magnetostatic interactions in rare-earth iron and rare-earth cobalt magnetic materials \([2,3,11,12]\). We have therefore neglected the stray field energy term in our model for simplicity. The magnetostatic energy density \( \phi_H \) is given by

\[
\phi_H = -\mu_0 \mathbf{H}_{\text{app}} \cdot \mathbf{M}_s(r),
\]

where \( \mathbf{H}_{\text{app}} \) is the applied magnetic field. Since, by definition, a system in remanent state entails \( H_{\text{app}} = 0 \), we thus get \( \phi_H = 0 \). It should be pointed out, however, while we set \( H_{\text{app}} = 0 \) for convenience in order to study a particular (remanent) state in the hysteresis loop, this state is obtained historically by applying and then removing an applied magnetic field. The distribution of the spontaneous magnetization, \( \theta(r) \) and \( \psi(r) \), is related to the applied magnetic field direction. So the magnetic moment directions as well as the orientation of the local easy axis \( \alpha(r) \) (see Fig. 1) are defined relative to the direction of the applied magnetic field. The term ‘applied field’ in the following refers to the historic external magnetic field.

According to the preceding discussions, we may write the total Gibbs free energy in terms of the exchange and the anisotropy energy, namely,

\[
\Phi_G = \int \left\{ A [ (\nabla \theta(r))^2 + (\nabla \psi(r))^2 \sin^2 \theta(r) ] + K \sin^2 \varphi(r) \right\} \, dr.
\]  

(2.7)

While the orientation of magnetization in the grain center is mainly determined by the anisotropy energy, the distribution of the magnetization near the grain boundaries is influenced by the exchange energy and is responsible for the remanence enhancement. In order to lower the total energy, the magnetic moments near the boundaries will point to directions which gradually change from the easy axis direction of one grain to that of a neighboring grain, while those in the grain center point in the direction of the easy axis, as shown in Fig. 2 for a plane isotropic easy axis distribution.

Our analytical model differs from the SW model in some important respects. In the SW model, the
magnetization curve of an aggregation of single domain particles is described by a uniaxial anisotropy due to either the particle shape or the magnetocrystalline anisotropy. For an isolated particle of crystal anisotropy $K$ and saturation magnetization $M_S$ in an applied field $H_{app}$, the total energy density is given by

$$E = K \sin^2(z - \theta) - \mu_0 H_{app} M_S \cos \theta. \quad (2.8)$$

In remanent state, the second term vanishes, and at equilibrium, the spontaneous magnetization $M_S$ points in the easy axis direction. For an assembly of non-interacting single domain particles with random orientations of easy axes, it yields a value of 0.5 for the ratio of the remanent magnetization $M_r$ to the saturation magnetization $M_S$. According to the SW model, the magnetization within a grain is completely determined by the easy axis, and the magnetization changes abruptly at the grain boundaries. In our model, however, a transition region is formed due to the exchange interactions between neighboring grains. The orientation of the magnetization changes smoothly in the transition region, from the easy axis direction of one grain to that of the neighboring grain (see Fig. 2).

Since the exchange interaction is limited to neighboring grains only, we shall first consider the remanence of a two-grain system (Fig. 2), and then generalize the results to a (one-dimensional) linear array of grains with in-plane easy axis distribution. In Section 4 this one-dimensional model is extended to a system with three-dimensional easy axis distribution where each grain has six neighbors.

3. Remanence enhancement of a chain of grains

The system studied in this section is a chain of infinite number of identical cubes (magnetic grains) with a cube length of $L$ (the grain size in this case). Each cube is connected to two other cubes (left and right). For simplicity, we solve an isotropic plane problem. All easy axes of the grains and the magnetic moments are restrained to the same $y$-$z$ plane. The magnetization is set to be uniform in the $x$-$z$ plane. The angle between an easy axis and the applied magnetic field direction, $z$, is a random number ranging from $-\pi/2$ to $\pi/2$. While the magnetization in the grain center is determined by the SW model, the magnetic moments in the grain boundaries change continuously with $y$, as shown in Fig. 2. Thus, setting $\psi(r) = \pi/2$ (corresponding to the $y$-$z$ plane) and $\varphi(r) = z(r) - \theta(r)$, Eq. (2.7) reduces to

$$\Phi_y = \int \left\{ A(\nabla \theta(r))^2 + K \sin^2[z(r) - \theta(r)] \right\} dy. \quad (3.1)$$

Since we consider the magnetic moments to change from one axis direction to the other as a function of only the $y$-coordinate, the magnetization distribution in the grain boundary is essentially a one-dimensional problem.

In order to demonstrate remanence enhancement as due to the exchange interactions in the grain boundaries, let us first consider and compare the remanence of two cubes using Eq. (3.1) with the result of the SW model. The magnetization orientation of the first half of the cube is determined by the interaction between this and the left cube, while the orientation of magnetization of the second half is determined by the interaction with the right cube. Therefore, the integration interval for the remanence of a two-cube system is chosen to be $-L/2$ to $L/2$. Because of translational symmetry in the $x$- and $z$-directions, Eq. (3.1) may be reduced to

$$\Phi_y = \int_{-L/2}^{L/2} \left\{ A(\nabla \theta(r))^2 + K \sin^2[z(r) - \theta(r)] \right\} dy. \quad (3.2a)$$

As mentioned before, $\theta(r)$ and $z(r)$ are the polar coordinates describing the directions of the spontaneous magnetization $M_S(r)$ and the easy axis direction, respectively. $\Phi_y$ is the Gibbs free energy per unit area for a two-grain system. Since no negative component of magnetization is expected at the remanent state in the positive $z$-direction after magnetization, the ranges of orientations of the spontaneous magnetization $\theta(r)$ and the local easy axis direction $z(r)$ are chosen between $-\pi/2$ and $\pi/2$. Thus, angles $-\pi/2$, 0, and $\pi/2$ correspond to the negative $y$-, positive $z$-, and positive $y$-direction, respectively (see Fig. 2). We consider two grains with easy axes $z_1$ and $z_2$, respectively. Without loss of generality, we set $-\pi/2 \leq z_1 \leq z_2 \leq \pi/2$, as
shown in Fig. 2. Grains 1 and 2 are on the left (with \( y < 0 \)) and on the right side (with \( y > 0 \)), respectively.

The magnetization in the grain center is given by the SW model. In remanent state, the magnetic moments in the grain centers orient along the respective easy axis directions so that we have

\[
\theta = x_1 \quad \text{for} \quad y = -L/2, \quad (3.2b) \\
\theta = x_2 \quad \text{for} \quad y = L/2. \quad (3.2c)
\]

Eq. (3.2a), (3.2b) and (3.2c) is analogous to a one-dimensional domain wall problem if the anisotropy energy is continuous in the grain boundary, which should be true from the point of view of symmetry. (The symmetry gives \( \theta = (x_1 + x_2)/2 \) at \( y = 0 \).) The exchange interaction in grain boundaries leads to a continuous change of direction of magnetization. Minimization of the total free energy of Eq. (3.2a) leads to the well-known Euler equation plus a surface constraint for the orientation of magnetization \( \theta \). Just as in the Bloch wall situation, the Euler equation and the surface constraint can be written as

\[
A_0 \frac{d\theta}{dy} = \pm \sin(x - \theta), \quad (3.3)
\]

where \( A_0 = \sqrt{A/K} \) is the so-called exchange length [2,3], and \( \delta_w = \pi A_0 \) is the Bloch wall width for 180° domain wall. For Nd\(_2\)Fe\(_{14}\)B, the Bloch wall width is 4.2 nm [2,3]. Grain sizes of Nd\(_2\)Fe\(_{14}\)B-based nanocrystalline materials are normally larger than 10 nm [2–7,18].

Eqs. (3.2b), (3.2c) and (3.3) compose a group of equations that define an equilibrium magnetization distribution in grain boundaries. Because the grain size is generally very large compared with the exchange length, we may set \( L = \infty \) in the boundary conditions of Eqs. (3.2b) and (3.2c) for mathematical simplicity. We will show later that this assumption is reasonable. Thus, we arrive at the following equations for the grain boundary of grains 1 and 2, namely,

\[
A_0 \frac{d\theta}{dy} = \pm \sin(\theta - x) \quad \text{for} \quad -\infty < y < +\infty, \quad (3.4a)
\]

\[
\theta = x_1 \quad \text{for} \quad y = -\infty, \quad (3.4b) \\
\theta = x_2 \quad \text{for} \quad y = \infty, \quad (3.4c)
\]

where \( x = x_1 \) for \( y \leq 0 \) and \( x = x_2 \) for \( y \geq 0 \) in Eq. (3.4a). By solving Eqs. (3.4a), (3.4b) and (3.4c), it can be shown that the angular distribution of \( M_\parallel(y) \) is given by

\[
\tan\left(\frac{\theta - x_1}{2}\right) = \tan\left(\frac{x_2 - x_1}{4}\right) \exp(y/A_0) \\
\text{for} \quad y < 0 \quad \text{(grain1)}. \quad (3.5)
\]

An analogous treatment for grain 2 leads to

\[
\tan\left(\frac{x_2 - \theta}{2}\right) = \tan\left(\frac{x_2 - x_1}{4}\right) \exp(-y/A_0) \\
\text{for} \quad y > 0 \quad \text{(grain2)}. \quad (3.6)
\]

Both Eqs. (3.5) and (3.6) lead to the same result that \( \theta = (x_1 + x_2)/2 \) at \( y = 0 \), indicating that the magnetic anisotropy energy is continuous at \( y = 0 \). This confirms that the assumptions leading to Eqs. (3.2a), (3.2b), (3.2c) and (3.3) are reasonable.

A typical distribution of magnetic moment orientation \( \theta \) is shown in Fig. 2, and the component of the reduced magnetization \( \cos \theta \) in the direction of the applied magnetic field (z-axis) is shown in Fig. 3 as a function of \( y \) for various easy axis orientations. In the transition region, the magnetic moment orientation \( \theta \) always lies between \( x_1 \) and \( x_2 \). The magnetic moment orientation approaches the easy axis orientation beyond about 5 nm from the grain boundary, confirming the validity of our treatment for grain size larger than 10 nm.

The figure further reveals that remanence enhancement is most effective when \( \theta_1 = -\theta_2 \), especially if \( \theta_1 = -\theta_2 = -\pi/2 \) (see Fig. 3a), where \( \cos \theta \) in the transition region is always larger than that in the center of the grain. Indeed, exchange interaction between neighboring grains always leads to remanence enhancement, the degree of which being dependent only on the orientations of the easy axes. Note that we define remanence enhancement \( \zeta \) as

\[
\zeta = M_r/M_{r,w} - 1, \quad (3.7)
\]

where \( M_{r,w} \) is the remanence predicted by the SW model.
Fig. 3. The magnetic moment orientation $\theta$ (solid line) and the corresponding $\cos \theta$ (dashed line) of a two-grain system are shown as a function of position (where $y$ is in units of $D_0$) for (a) $\theta_1 = -\pi/2$ and $\theta_2 = \pi/2$, (b) $\theta_1 = -\pi/4$ and $\theta_2 = \pi/4$, (c) $\theta_1 = 0$ and $\theta_2 = \pi/2$, and (d) $\theta_1 = 0$ and $\theta_2 = \pi/4$. The grain boundary is at $y = 0$.

The remanence of a two-grain system, $M_r^{two}$, can be obtained by averaging $M_S \cos \theta$ from $-L/2$ to $L/2$, where $L$ is the grain size. It is given by

$$\frac{M_r^{two}}{M_S} = \frac{1}{M_S L} \int_{-L/2}^{L/2} M_S \cos \theta \, dy$$

$$= \frac{1}{2} (\cos \alpha_1 + \cos \alpha_2)$$

$$+ \frac{A_0}{2L} (\sin \alpha_2 - \sin \alpha_1)(\alpha_2 - \alpha_1)$$

$$- \frac{A_0}{L} (\cos \alpha_1 + \cos \alpha_2)$$

$$\times \ln \left[ 1 + \tan^2 \left( \frac{\alpha_2 - \alpha_1}{4} \right) \right] + O(M),$$

where the dimensionless $O(M)$ is given by

$$O(M) = - \frac{2A_0}{L} \left( \sin \alpha_2 - \sin \alpha_1 \right) \tan^{-1}$$

$$\times \left[ \tan \left( \frac{\alpha_2 - \alpha_1}{4} \right) \exp \left( - \frac{L}{2A_0} \right) \right]$$

$$+ \frac{A_0}{L} (\cos \alpha_1 + \cos \alpha_2)$$

$$\times \ln \left[ 1 + \left[ \tan \left( \frac{\alpha_2 - \alpha_1}{4} \right) \exp \left( - \frac{L}{2A_0} \right) \right]^2 \right].$$

(3.8)
Due to the factor $\exp[-L/(2A_0)]$, $O(M)$ is much smaller than one, and can thus be neglected. For instance, using Nd$_2$Fe$_{14}$B as a test case where $A_0 \approx 1.34$ nm and $L \approx 10$ nm, we obtain $O(M) < 0.01$.

The first term in Eq. (3.9), $(\cos \alpha_1 + \cos \alpha_2)/2$, expresses the reduced remanence predicted by the SW model, which is $2/\pi$ for a plane problem and 0.5 for a three-dimensional easy axis distribution. The second term represents the remanence enhancement due to exchange interaction, and is always positive. Thus, our calculated remanence is always greater than that predicted by SW model. The remanence enhancement is most effective when $\alpha_1 = -\alpha_2$ and the maximum enhancement is obtained when $\alpha_1 = -\pi/2$ and $\alpha_2 = \pi/2$. Contribution from the third term is less than 0.015 for the NdFeB magnet, and it will be excluded from further discussion. The reduced remanence of a two-grain system with easy axis orientations $\alpha_1$ and $\alpha_2$ (where $\alpha_1 \leq \alpha_2$) is thus given by

$$\frac{M_r^{\text{two}}}{M_s} = \frac{1}{2}(\cos \alpha_1 + \cos \alpha_2) + \frac{A_0}{2L}(\sin \alpha_2 - \sin \alpha_1)(\alpha_2 - \alpha_1). \quad (3.11)$$

The calculated reduced remanence for a two-grain Nd$_2$Fe$_{14}$B system, according to Eq. (3.11), is shown in Fig. 4 as a function of grain size for various easy axis orientations.

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Fig. 4. The remanence enhancement of a two-grain Nd$_2$Fe$_{14}$B system is shown as a function of grain size (in units of $A_0$) for (a) $\theta_1 = -\pi/2$ and $\theta_2 = \pi/2$, (b) $\theta_1 = -\pi/4$ and $\theta_2 = \pi/4$, (c) $\theta_1 = 0$ and $\theta_2 = \pi/2$, and (d) $\theta_1 = 0$ and $\theta_2 = \pi/4$. The dashed line denotes the predictions of the SW model.
Fig. 5. The remanence enhancement is shown as a function of grain size for a chain of cubic grains. The solid line, dashed line and the solid circle denote the present results, the finite-element calculations [3] and the experimental measurements [7], respectively.

axis orientations. The figure reveals that remanence increases with decreasing grain size. Although there is little remanence enhancement for grain size larger than 50Å, it increases rapidly for sizes smaller than 40Å (or about 13 Bloch wall widths).

Integrating Eq. (3.11) over all possible \( x_1 \) and \( x_2 \), we obtain the reduced remanence of a chain of magnetic grains as

\[
\frac{M_t}{M_S} = \frac{2}{\pi} \left( 1 + \frac{A_0}{L} \right),
\]

(3.12)

According to Eq. (3.7), remanence enhancement for this system is thus given by

\[
\zeta = \frac{A_0}{L}.
\]

(3.13)

In Fig. 5, we show the calculated remanence enhancement of Nd\(_2\)Fe\(_{14}\)B with \( A_0 = 1.34 \) nm, together with the result of a finite-element study [3] and the experimental measurement [7] for comparison. Overall good agreement between calculated and measured remanence enhancement is obtained. However, our calculations consistently underestimate the enhancement, the reason being that our model is one-dimensional as opposed to, for instance, the two-dimensional model of the finite-element approach.

4. Three-dimensional remanence enhancement

In a three-dimensional problem, the easy axes and applied magnetic field are not necessarily in the same plane. In this case, the Gibbs free energy given in Eq. (2.7) can still be minimized to determine the magnetization distribution and thus the remanence enhancement. However, the problem becomes so complicated that an analytical solution cannot be easily obtained. Instead, we will estimate the remanence enhancement based on the following arguments. Since only the orientations of the magnetizations and the easy axes are significant in determining the remanence, while the actual locations of these magnetic moments and easy axes are unimportant, we may shift the easy axis of one grain towards the easy axis of a neighboring grain so that the two easy axes lie in a plane (Fig. 6). The magnetizations in the transition region between these two grains are distributed in various directions in the same plane, between those of the easy axes. We then obtain the average magnetization by dividing the vector sum of the magnetizations by the grain size \( L \). The net remanence for this grain boundary can then be obtained by simply projecting the average magnetization along the direction of the applied magnetic field. Integrating this net remanence over all possible easy axis directions yields the macroscopic remanence and remanence enhancement.

Suppose the angle between the easy axes of two neighboring grains specified by \((x_1, \beta_1)\) and \((x_2, \beta_2)\) is \( \delta \) (see Fig. 6). Then

\[
\cos \delta = \cos x_1 \cos x_2 + \sin x_1 \sin x_2 \cos(\beta_2 - \beta_1).
\]

By symmetry, the total magnetization lies in the direction that bisects the angle \( \delta \). It can be shown that the angle \( \sigma \) between the total magnetization

\[
= \frac{2}{\pi} \left( 1 + \frac{A_0}{L} \right).
\]
and the applied magnetic field is given by

$$\cos \sigma = \frac{\cos \alpha_1 + \cos \alpha_2}{2 \cos(\delta/2)}. \quad (4.1)$$

The magnitude of the total magnetization $M_{\text{total}}$ can be obtained from the results of the plane problem. Using $\alpha_1 = -\delta/2$ and $\alpha_2 = \delta/2$ in Eq. (3.11), we get

$$\frac{M_{\text{total}}}{M_S L} = \cos \left(\frac{\delta}{2}\right) + \frac{A_0}{L} \cos \left(\frac{\delta}{2}\right). \quad (4.2)$$

The net remanence $M_{\text{net}}$, the projection of the average magnetization along the direction of the applied magnetic field, is given by

$$M_{\text{net}} = M_{\text{total}} \cos \sigma / L. \quad (4.3)$$

Integrating the above equation over all possible easy axis directions will give the macroscopic remanence as

$$M_r = \int_{0}^{\pi/2} \sin \alpha_1 \int_{0}^{\pi/2} \sin \alpha_2 \int_{0}^{2\pi} d\beta_1 \int_{0}^{2\pi} d\beta_2 M_{\text{net}} d\beta_2,$$

$$= \int_{0}^{\pi/2} \sin \alpha_1 \int_{0}^{\pi/2} \sin \alpha_2 \int_{0}^{2\pi} d\beta_1 \int_{0}^{2\pi} d\beta_2 M_{\text{net}} d\beta_2.$$

(4.4)

The integration is carried out numerically and the following result is obtained:

$$M_r / M_S = 0.5 + 0.6 \Delta_0 / L. \quad (4.5)$$

The constant term on the right-hand side corresponds to the bulk contribution (as given by the SW model), and the second term reflects the contribution from the grain boundaries.

In a normal 3D material every cubic grain has six neighboring grains. For grains that are much larger than the Bloch wall width, the grain boundary area is three times of that of a grain in a chain, and the remanence enhancement is thus expected to be three times larger. In view of this consideration, a prefactor of three is multiplied into the second term of Eq. (4.5) to give the reduced remanence in 3D as

$$M_r / M_S = 0.5 + 1.8 \Delta_0 / L. \quad (4.6)$$

Similar to the case of in-plane easy axis distribution, the remanence enhancement is inversely proportional to the grain size $L$ and significant remanence enhancement occurs when the grain size $L$ is less than $18 \Delta_0$, or about 6 Bloch wall widths. The corresponding remanence enhancement is about 20%. When the grain size is $7 \Delta_0$, the reduced remanence is 0.76, which is 50% larger than that predicted by the SW model.

The calculated grain size dependence of remanence enhancement for our test Nd$_2$Fe$_{14}$B system is shown in Fig. 7, in comparison with the empirical relationship derived from the finite-element calculations [2], namely,

$$J_r = J_{\text{sat}}[0.6854 - 0.0454 \ln(D/\delta_{\text{hard}})], \quad (4.7)$$

where $J_r = \mu_0 M_r$ and $J_{\text{sat}} = \mu_0 M_S$ is the remanent polarization and saturation polarization, respectively. $D$ is the grain diameter, which is equivalent to $L$ in our model, and $\delta_{\text{hard}}$ is the Bloch wall width given by $\pi \Delta_0$. Good agreement is obtained between the two approaches, in particular for grain size larger than 20 nm. For smaller grains (less than 20 nm), however, the discrepancy is larger, the reason being that our model is valid only for grain size much larger than the Bloch wall width (or about 4.2 nm in our present example).
5. Conclusions

Based on a simple micromagnet approach, we have derived an analytical expression for remanence enhancement for a chain of grains, in which the easy axis distribution is assumed to be plane isotropic, and then generalizing it for a three-dimensional array of grains. Application of the formulae to Nd$_2$Fe$_{14}$B system demonstrates good overall agreement with available experimental and other theoretical studies. Our analysis shows that remanence enhancement increases with Bloch wall width but decreases with grain size, and that remanence is particularly enhanced at the grain boundaries.

References