Micromagnetic simulations of demagnetization curves for single-phase nanocrystalline PrFeB magnet

X.P. Wang[a,*], S.F. Zhao[b], X.F. Han[b]

[a]*Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong*
[b]*State Key Laboratory of Magnetism, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China*

Dedicated to Roderick S.C. Wong on the occasion of his 60th birthday

Abstract

The Gauss–Seidel projection method developed in [E. Weinan, X.P. Wang, SIAM J. Numer. Anal. 38 (2000) 1647–1665 and X.P. Wang, C.J. Garcia-Cervera, E. Weinan, J. Comp. Phys. 171 (2001) 357] is used to calculate the demagnetization curves for the single-phase nanocrystalline PrFeB magnet. It is observed that magnetic reversal for PrFeB magnet starts near the grain boundary where the angle between the external magnetic field and easy direction of the magnet can be as large as 90°. We also calculated the demagnetization curves, coercivity $\mu_0 H_c$ and remanence J_r for different temperatures. The numerical results are consistent with the experimental observations. © 2005 Elsevier B.V. All rights reserved.

1. Introduction

The magnetic properties of nanocrystalline PrFeB magnets are as good as the NdFeB magnet. They give better performance in lower temperature than in room temperature due to their lack of spin reorientation which can lead to significant reduction of the maximum energy product, as in the case of NdFeB magnets. Recent research [9,3,6,1] has demonstrated that nanocrystalline PrFeB permanent magnets have high coercivity $\mu_0 H_c$ even in low temperature. The remanence may be enhanced remarkably, leading to a

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* Corresponding author.
  E-mail address: mawang@ust.hk (X.P. Wang).

significant increase of the maximum energy production. In [6], a formula for coercivity $\mu_0 H_c$ was derived which gives the relation of $\mu_0 H_c$ to several material and microstructure parameters. The demagnetization curves for nanocrystalline PrFeB magnets at different temperatures are calculated in [9]. However, the results are only qualitative compared to the experiments. For example, the error in $\mu_0 H_c$ is close to 100% compared to the experimental value.

It is observed by Jin et al. [5] in their simulation of nanocrystalline NdFeB magnets that if the number of grains N is not enough (e.g., between 30 and 90), the calculated demagnetization curves are very sensitive to the direction of the external field. The calculated $\mu_0 H_c$ also varies with the direction of the external field. However, this dependence of $\mu_0 H_c$ on the direction of the external field can be reduced by increasing the number of grains. This partly explains the deviation of the numerical results in [9] from the experimental values. Constrained by the computational cost, the number of grains used in [9] is only $N = 64$, which is not enough to give accurate results.

Numerical simulation based on the Landau–Lifshitz–Gilbert (LLG) equation has been used to study both static and dynamic issues related to magnetic materials and to characterize the magnetic behavior of such different materials as thin film heads, recording media, patterned magnetic elements, magnetic tunnel junction, MRAM and nanocrystalline permanent magnets [10,15,8,9,13,2]. In [14,11], an unconditionally stable scheme is developed for the Landau–Lifshitz–Gilbert equation. This method is based on a combination of a Gauss–Seidel implementation of a fractional-step implicit solver for the gyromagnetic term, and the projection method for the damping term. The method is shown to speed up the simulation significantly and allows them to carry out fully resolved calculations for the switching of the magnetization in micron-sized elements in a two-dimensional setting [11] and for three-dimensional cross-tie wall structures [12].

In this paper, we use the Gauss–Seidel projection method for LLG equations to simulate the demagnetization curves for nanocrystalline PrFeB magnets with larger total number of grains. It is observed that magnetic reversal for PrFeB magnet starts near the grain boundary where the angle between the external magnetic field and easy direction of the grain can be as large as 90°. We also calculated the demagnetization curves, coercivity $\mu_0 H_c$ and remanence J_r for different temperatures. The numerical results are consistent with the experimental observations.

2. Simulation model

The dynamics of magnetization distribution is obtained from the LLG equation

$$\mathbf{M}_t = -\gamma \mathbf{M} \times \mathscr{H} - \frac{\gamma \alpha}{M_s} \mathbf{M} \times (\mathbf{M} \times \mathscr{H}), \tag{1.1}$$

where $|\mathbf{M}| = M_s$ is the saturation magnetization, and is usually set to be a constant far from the Curie temperature. The first term on the right-hand side is the gyromagnetic term, with γ being the gyromagnetic ratio. The second term on the right-hand side is the damping term, with α being the dimensionless damping coefficient. $\mathscr{H}$ is the local effective field, computed from the Landau–Lifshitz free energy functional:

$$\mathscr{H} = -\frac{\delta G}{\delta \mathbf{M}}. \tag{1.2}$$