Physica B 449 (2014) 214–219

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Size-dependent exchange bias in ferromagnetic (core)/antiferromagnetic (shell) nanoparticles

Yong Hu [a,*], Yan Liu [a], Hai-Na Wu [a], An Du [a], Feng Shi [b]

[a] College of Sciences, Northeastern University, Shenyang 110819, China
[b] Physics Department, Auburn University, AL 36849, USA

ARTICLE INFO

Article history:
Received 9 August 2013
Received in revised form
16 March 2014
Accepted 13 May 2014
Available online 2 June 2014

Keywords:
Nanoparticle
Exchange bias
Magnetization reversal
Microscopic spin configuration
Antiferromagnetic anisotropy
Monte Carlo simulation

ABSTRACT

We report a numerical study of the dependence of exchange bias on ferromagnetic core/antiferromagnetic shell dimension in an isolated nanoparticle, on the basis of a modified Metropolis Monte Carlo simulation. A pronounced exchange bias field is obtained at a finite size of ferromagnetic core radius, while the value of exchange bias field decreases monotonously up to a lower stable value with further increasing core sizes. Due to the complex core/shell structure and the mode conversion of magnetization reversal for various core sizes, the dependence of exchange bias field on the ferromagnetic component size is different from that in planar systems. Moreover the exchange bias field can be stabilized above a certain antiferromagnetic shell thickness, where the effective anisotropy of the whole antiferromagnetic shell becomes strong enough. It has been demonstrated unambiguously how the core and shell dimensions optimize the exchange bias.

1. Introduction

Recently, much attention has been paid to magnetic nanoparticles, arising from current and foreseen applications [1]. Research works on bimagnetic nanoparticles, where both shell and core are magnetic, are steadily increasing, particularly since the report on the use of exchange bias (EB) to beat the superparamagnetic limit in ultrahigh-density magnetic recording media or to enhance the magnetic hardness in permanent magnets [2,3]. The EB, which commonly causes a shift of ferromagnetic (FM) hysteresis loop, is a consequence of the direct exchange at the interface between FM and antiferromagnetic (AFM) layers and/or nanoscale heterostructures. Despite a half of century having elapsed since its discovery [4], there is still a disparity between experimentally obtained values for EB field (H_E) and those predicted by simple theories.

Different from planar systems, control of EB through varying an FM or AFM dimension independently in bimagnetic nanoparticles is a significant technical challenge experimentally. To highlight the EB, FM and AFM components need to be kept single-domain and in the vicinity of their interface a high crystallization is also required. Moreover, the FM and AFM dimensions must be not only controllable but also monodisperse and distinguishing for the accurate measurement [5]. However, the spherical interface between FM and AFM components always tends to result in an intrinsic disorder and a finite-size effect in spin arrangements [6]. Therefore, a numerical study is necessary to demonstrate the puzzled issue on how to optimize the EB by means of the core/shell dimension in nanoparticles.

2. Model and Monte Carlo simulation

A model of an isolated nanoparticle with an FM (core)/AFM (shell) morphology is exploited, and its radius can vary from 6.5a to 15.0a through increasing the core/shell dimension meanwhile keeping the other constant where a is the lattice constant. Simple cubic crystal packing is used, and thus the maximum coordination number of spin is six. Besides the regions of FM core, AFM shell, and their interface an outer surface region, where every spin has at least one dangling bond, is also defined due to its magnetic properties that are different from those of the bulk (including a larger anisotropy and a random spin orientation) [7–9]. The large surface anisotropy originates from the broken symmetry on the surface, surface–core strains, and magnetostriction, while also because of the lower coordination of spins on the surface the exchange interaction on or around the surface is in general weaker than that in the bulk [10,11].

The Heisenberg-type Hamiltonian of the whole system under an external magnetic field (H) can be written as

$$H = -J_C \sum_{<i,j \in \mathrm{FMcore}>} S_i \cdot S_j - J_{SH} \sum_{<i,j \in \mathrm{AFMshell}>} S_i \cdot S_j - J_{IF}$$

* Corresponding author. Tel.: +86 24 8368 7658; fax: +86 24 8367 8686.
E-mail address: huyong@mail.neu.edu.cn (Y. Hu).

http://dx.doi.org/10.1016/j.physb.2014.05.035
0921-4526/

$$\sum_{<i\in \text{FMcore}, j\in \text{AFMshell}>} S_i\cdot S_j - J_{SU} \sum_{<i \text{or} j\in \text{surface}>} S_i\cdot S_j - \sum_{i\in \text{FMcore}} K_C(S_i\cdot\hat{z})^2 - \sum_{i\in \text{AFMshell}} K_{SH}(S_i\cdot\hat{z})^2 - \sum_{i\in \text{surface}} K_{SU}(S_i\cdot\hat{n})^2 - H\cdot\sum_i S_i, \quad (1)$$

where S_i, S_j are atomic spins at sites i and j. The first line in Eq. 1 gives the exchange interactions between the nearest-neighbor spins belonging to the FM core, AFM shell, FM/AFM interface, and surface, with the exchange coupling constants $J_C = 1.0$, $J_{SH} = -0.2$, $J_{IF} = -0.2$, and $J_{SU} = -0.1$. Then the anisotropies of spins in the FM core, AFM shell, and surface are described in the second line, with the anisotropy constants $K_C = 0.02$, $K_{SH} = 1.0$, and $K_{SU} = 1.4$, as discussed above. In addition we suppose that the core/shell anisotropy is uniaxial along the z axis while, to simulate the disordered configuration on the surface, the surface anisotropy is specified to be normal to the surface at every site, in a direction calculated from the surface neighbor positions. If the unit of exchange coupling constant is equivalent to 10^3 K, the J_C corresponds to a Curie temperature $T_C \sim 0.725ZJS^2/3$ of 1450 K and J_{SH} corresponds to a Néel temperature (T_N) of 290 K. The values are similar to those of Co/CoO nanoparticles ($T_C = 1388$ K and $T_N = 290$ K in Ref. [12]). Finally a Zeeman energy, where the H is also applied along the z axis, is added in the last term of Eq. 1. It is noteworthy that we neglect dipolar interactions, since their role is less pronounced than anisotropies due to the relatively small size of nanoparticles.

A modified Metropolis Monte Carlo simulation, which has been used previously [13–16], is performed to update the spin orientation. In the simulation a disordered core/shell nanoparticle system is firstly cooled from a high temperature $T_0 = 1.0$ to a desired $T = 0.01$ under an external magnetic field $H_{FC} = 1.5$, which is strong enough to saturate the system. At the second stage, the hysteresis loop is recorded by cycling the H from 0.5 to -0.5 to extract the H_E. The magnetization is averaged over a number of 10^4 Monte Carlo steps per spin after another 10^4 Monte Carlo steps per spin used for thermalization.

3. Results and discussion

Firstly, the radius of FM core (R_{FM}) is varied from $0.5a$ to $9.0a$ in the core/shell nanoparticle with a fixed thickness of AFM shell ($t_{AF} = 6.0a$), and their hysteretic behaviors after field cooling are measured to study the EB phenomenon. Fig. 1(a) plots the values of H_E versus R_{FM} between $2.5a$ and $9.0a$. Meanwhile, Fig. 1(c) shows some hysteresis loops of the FM core with some representative R_{FM}. Smaller FM cores ($R_{FM} < 2.5a$) cannot form a closed hysteresis loop and thus fail to extract a valid H_E. They are therefore excluded in Fig. 1. For $R_{FM} \geq 2.5a$ the H_E is positive and decreases monotonously with increasing R_{FM} and, finally, levels out. That is, the hysteresis loop shifts towards the positive field direction. In particular two branches of the hysteresis loops for small R_{FM} ($< 3.5a$) both intersect the field axis at positive field values, seldom observed experimentally. It is well known that Nogués et al. [17] applied a strong H_{FC} on the Fe/FeF_2 bilayers with an AFM J_{IF}, and first observed the positive EB phenomenon. Two necessary conditions are also satisfied here, and the positive H_E appears undoubtedly. Next, we focus on the interpretation of the hysteretic behaviors for various R_{FM} and the dependence of H_E on R_{FM}.

In general it is accepted that EB is an interfacial effect in FM/AFM systems [18], and the magnetization behavior of the AFM component at the interface may play a significant role in establishing the EB. On the other hand H_E is always quantified by the values of coercive field, called as switching field in the FM hysteresis loop,

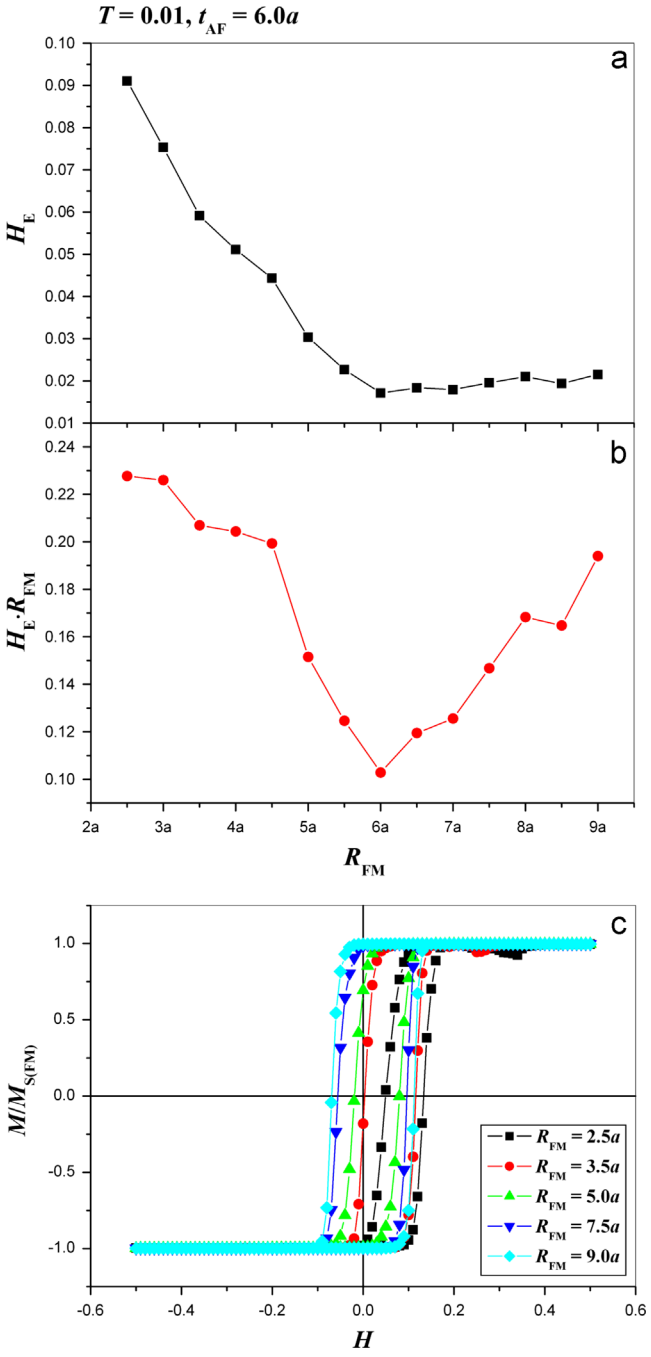

Fig. 1. (a) Exchange bias field and (b) product of the exchange bias field and ferromagnetic core radius as functions of the core radius. (c) Ferromagnetic hysteresis loops for the representative core radii, where $M_{S(FM)}$ is a saturated value of ferromagnetic magnetization.

where the magnetization reverses are governed by a reversal mode. Hence, the study on the magnetization reversal mode will help estimate the values of coercive field and finally demonstrate the EB behaviors [19–21]. Accordingly, the magnetization behaviors of the AFM shell at the interface as well as the microscopic spin configurations of the nanoparticles with a large and a small FM core during magnetization reversal are presented in Figs. 2 and 3, respectively. As shown in Fig. 2(a), when the H becomes weak, the magnetization of the AFM shell at the interface drops to a lower value from its saturated value because the AFM spins at the FM/AFM interface are rearranged mainly due to the J_{SH}. However, the magnetization cannot be offset completely and a nonzero surplus