Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Numerical study of exchange bias in antiferromagnetic/ferromagnetic core/shell nanoparticles with non-magnetic defects

Z.D. Vatansever

Department of Physics, Dokuz Eylül University, Tr-35160 İzmir, Turkey

ARTICLE INFO

Article history:
Received 26 May 2018
Received in revised form 26 June 2018
Accepted 2 July 2018
Available online xxxx
Communicated by M. Wu

Keywords:
Core/shell magnetic nanoparticles
Exchange bias
Monte Carlo simulation

ABSTRACT

We perform Monte Carlo simulations for an antiferromagnetic/ferromagnetic core/shell nanoparticle with a doubly inverted structure. We investigate the dependence of the exchange bias field and coercivity on the magnetic dilution of the shell-interface and shell part. It is demonstrated that exchange bias and coercivity can exhibit monotonic or non-monotonic behavior depending on the location of the non-magnetic components. Also, temperature dependence of the exchange bias and coercivity of the system are studied for a particular defect concentration value. Our results provide an alternative way for tunning the magnetic properties of doubly inverted nanoparticles.

1. Introduction

The phenomenon of exchange bias (EB) typically occurs when a ferromagnetic (FM) material is in contact with an antiferromagnetic (AFM) material after cooling the system below the Néel temperature (T_N) of the AFM [1–3]. Although EB phenomenon was discovered about five decades ago in Co/CoO nanoparticles [4,5], it is still the focus of interest because of the usage of EB biased systems in several application areas, for instance magnetic recording media [6].

It is a well known fact that EB occurs due to the exchange interaction between the FM and AFM material. The net magnetization along the AFM interface remains pinned during the magnetization reversal which results in a shift in the hysteresis loop. According to the model introduced by Malozemoff [7–9], EB does not occur in a compensated FM/AFM interface and existence of EB is due to the interface's roughness. On the other side, it is demonstrated both experimentally and by Monte Carlo (MC) simulations that EB field can be observed as a result of the magnetic domains which are created by replacing magnetic atoms in the volume part of the AFM layer by non-magnetic atoms or defects [10–13]. In the case of core/shell nanoparticles, the FM/AFM interface has natural uncompensated spins because of the finite size and shape of the system even when the system does not contain any defects or roughness [14].

Recently, there has been an interest in investigating the EB effects by adding defects in FM/AFM interface [15–18]. For instance, effects of interface site and bond dilution on the EB properties of a system with a FM layer which is in contact with a diluted AFM layer have been studied by MC simulations [15]. A particular attention has been paid for the dilution in the FM interface and remarkably, an enhancement in EB field for small dilutions has been reported. Also, the EB and coercive field of a FM/AFM core/shell nanoparticle has been shown to exhibit monotonic or non-monotonic dependence on the concentration of non-magnetic atoms depending on the position of the defects [16]. These works provide a way to tune the EB field of the systems consisting of FM/AFM interfaces [15,16,19].

When an AFM material is located in the core part of the nanoparticle and it is covered by a FM or FiM material, a new type of system: inverted nanoparticle, can be obtained [20–28]. Inverted nanoparticles are categorized as "single-inverted" or "doubly inverted" depending on the relative transition temperatures of the core and shell components. In the case of single-inverted nanoparticles, Curie temperature (T_C) of the FM or FiM shell is higher than the Néel temperature (T_N) of the AFM core ($T_C > T_N$), such as FeO/Fe_3O_4 [29–32]. Doubly-inverted structures are the nanoparticles with $T_N > T_C$ as opposed to the traditional systems (e.g. MnO/Mn_3O_4 [20,25]). Location and relative transition temperature of the magnetic components in doubly inverted structures induces interesting behaviors including non-monotonic variation of the EB with AFM core radius [20,33] and existence of exchange bias fields above T_C [27].

In the present work, we model a doubly inverted nanoparticle system and consider a site dilution in FM part of core/shell interface as well as in the FM shell part. We investigate the effects of concentration of non-magnetic components on the EB field and

E-mail address: zeynep.demir@deu.edu.tr.

https://doi.org/10.1016/j.physleta.2018.07.001
0375-9601/

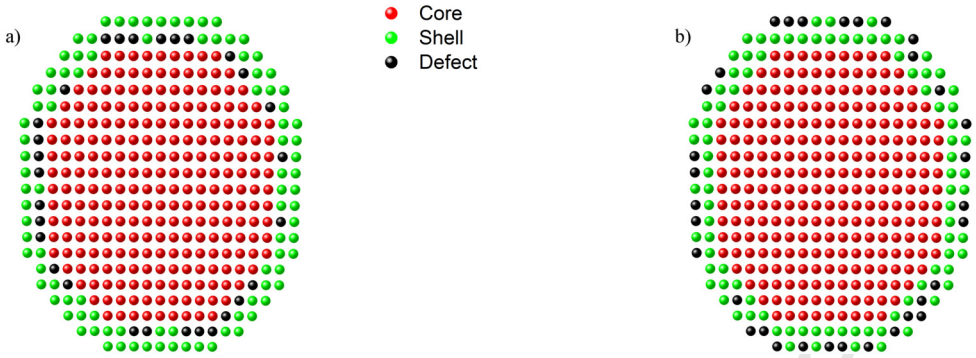

Fig. 1. (Color online.) Schematic representation of the core/shell nanoparticle when non-magnetic dilution is performed a) in the shell interface b) in the shell part of the system. The figures are shown for a defect concentration of 0.5.

coercivity of the system by MC simulations based on Metropolis algorithm which has been proven to be useful to understand EB microscopically in nanoparticles [14,34–39]. Besides, the temperature dependence of EB and coercivity are studied. Our numerical results indicate that introducing defects in FM shell part rather than the AFM core presents new physical consequences and an alternative way for tunning magnetic features of inverted structures.

The paper is organized as follows. In Section 2, we introduce the model Hamiltonian used for describing the inverted nanoparticle. Then, we give the details of the MC simulation procedure. Simulation results regarding the dependence of the EB and coercivity on the defect concentration and temperature are presented in Section 3. Finally, our brief summary is given in Section 4.

2. Model and method

We consider a spherical AFM/FM core/shell nanoparticle with a total radius of $R = 11a$ and a shell thickness of $t = 2a$ where a is the lattice constant as shown in Fig. 1. The spherical nanoparticle is obtained by cutting a sphere from an infinite simple cubic lattice. We describe the magnetic structure of the system by a classical Heisenberg Hamiltonian with a classical spin vector, $\vec{S}_i$, at site i:

$$\mathcal{H} = -J_c \sum_{\langle ij\rangle\, \epsilon\, core} \vec{S}_i \cdot \vec{S}_j - J_{sh} \sum_{\langle ij\rangle\, \epsilon\, shell} \vec{S}_i \cdot \vec{S}_j - J_{int} \sum_{\langle i\, \epsilon\, core, j\, \epsilon\, shell\rangle} \vec{S}_i \cdot \vec{S}_j - D_c \sum_{i\, \epsilon\, core} (S_i^z)^2 - D_{sh} \sum_{i\, \epsilon\, shell} (S_i^z)^2 - h \sum_{i}^{N} S_i^z. \quad (1)$$

Here, the first three sums are over the nearest neighbor spins and they correspond to exchange energy contribution from AFM core, FM shell and the coupling between core and shell, respectively. The spins of the AFM core are taken as $|\vec{S}| = 1$ while FM shell contains magnetic components with $|\vec{S}| = 3/2$. The external magnetic field is denoted as h and it is applied along the z direction. The exchange interaction constant in the shell is set to unity, $J_{sh} = 1$ and it is used as the unit of energy. The core/shell interface consists of core (shell) spins with at least one nearest neighbor in the shell (core). The interface coupling constant is taken as $J_{int} = J_{sh}$, namely ferromagnetic. Also, in order to model a doubly inverted nanoparticle with $T_N > T_C$ we set $J_c = -5J_{sh}$. We assume an uniaxial anisotropy along the z direction and take the anisotropy constants of core and shell parts as, $D_c = J_{sh}$ and $D_{sh} = 5J_{sh}$, respectively. It should be noted that the spin magnitudes of the magnetic components, exchange coupling, anisotropy parameters are chosen arbitrarily and they do not refer to a specific material.

As one can see from Fig. 1, we assume that the nanoparticle system is magnetically diluted. Namely, some of the lattice sites, which are selected randomly, are occupied by non-magnetic defects whose spin magnitudes are set to zero. Dilution process consists of two distinct procedures. In our first analysis, the non-magnetic defects are located only in the shell interface. While in the second analysis, the sites of FM shell are occupied by non-magnetic defects, however, the dilution is not performed in the shell interface. In order to simulate the hysteresis loops, we implement MC simulations with single spin-flip Metropolis algorithm [40,41]. The nanoparticle is cooled down in the presence of a cooling field, $h_{fc}/J_{sh} = 4$, from a reduced temperature of, $k_BT/J_{sh} = 10$, which is above the Néel temperature of the AFM core, to an interested lower temperature. Then, in order to complete the hysteresis loop, magnetic field from h/J_{sh} to $-h/J_{sh}$ and then from $-h/J_{sh}$ to h/J_{sh} with a magnetic field step of $\Delta h/J_{sh} = 0.05$ is applied which correspond to increasing and decreasing field branch, respectively. In every magnetic field step, numerical data are collected over 15×10^3 MC steps after discarding the first 5×10^3 MC steps for equilibration process.

We consider a quenched random disorder configuration means that the position of magnetic or non-magnetic components do not change during a simulation. For a specific disorder configuration, exchange bias and coercive fields are calculated as $H_E = -(H_{left} + H_{right})/2$ and $H_C = (H_{right} - H_{left})/2$, where H_{left} and H_{right} terms denote the coercive fields of the decreasing and increasing field branch, respectively. Average of the thermodynamic quantities are taken over 50 independent disorder realizations.

3. Results

3.1. Dilution in FM shell interface

In the following, we will discuss the dependence of the EB field and coercivity on the site dilution of the FM shell interface. Here, we denote the concentration of the non-magnetic ions by x_{int}. Simulation results for the typical hysteresis curves for the total magnetization, m_T, are presented in Fig. 2 for several concentration values. It is possible to observe that the clean case ($x_{int} = 0$), displays a loop shift which is compatible with both experimental [20,25,27] and theoretical [33] studies which indicate the existence of EB behavior in doubly inverted nanoparticles. On the other hand, for the system with full dilution of the shell interface ($x_{int} = 1.0$), the EB field is zero because the FM shell is completely separated from the AFM core. In the case of x_{int} values other than fully diluted state, the loop shift in hysteresis loops can be readily seen.

EB field as a function of the concentration of the non-magnetic ions in the FM shell interface is shown in Fig. 3. As expected, EB

Please cite this article in press as: Z.D. Vatansever, Numerical study of exchange bias in antiferromagnetic/ferromagnetic core/shell nanoparticles with non-magnetic defects, Phys. Lett. A (2018), https://doi.org/10.1016/j.physleta.2018.07.001