Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Tunning exchange bias in inverted antiferromagnetic/ferromagnetic core/shell nanoparticles by binary alloy shells

Z.D. Vatansever, E. Vatansever *

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

ARTICLE INFO

Article history:
Received 17 June 2018
Received in revised form 27 July 2018
Accepted 9 August 2018
Available online xxxx
Communicated by M. Wu

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

ABSTRACT

A detailed investigation of exchange bias properties of an inverted nanoparticle with an antiferromagnetic core and a ferromagnetic binary alloy shell of the type B_xC_{1-x} is presented by benefiting from Monte Carlo simulations. Exchange bias displays a non-monotonic behavior with the varying value of the concentration the type-B magnetic components, x. Coercivity exhibits a monotonic or a non-monotonic variation with x depending on the relative strength between unlike magnetic components in the shell. Particular attention has also been given to determine the effects of the cooling field process on the magnetic properties of the nanoparticle. Numerical results obtained in this work present a different physical mechanism and an alternative way for tuning the exchange bias and coercivity of bimagnetic core/shell nanoparticles.

1. Introduction

Exchange bias effects are typically observed when a material which is composed of a ferromagnetic (FM) and antiferromagnetic (AFM) interface is cooled from a temperature between the Curie temperature of FM material, T_C, and Néel temperature of AFM material, T_N ($T_N < T < T_C$), to a temperature below T_N ($T < T_N$) in the presence of a static magnetic field. During the cooling process, the exchange coupling at the FM/AFM interface induces unidirectional exchange anisotropy which brings about several interesting phenomena, for instance, loop shift in hysteresis (i.e., exchange bias) and coercivity enhancement [1–3]. The exchange bias was discovered in Co/CoO core/shell nanoparticles for the first time [4,5]. Since then, exchange bias and related properties have been investigated in many other bimagnetic nanoparticles including ferrimagnetic FiM/AFM [6], FM/FiM [7], FiM/FiM [8–10] core/shell systems because exchange coupled systems become efficient tools in several application areas for instance, enhancement of superparamagnetic blocking temperatures [11], permanent magnets [12,13] and magnetic recording media [14].

Recently, there has been a growing interest in inverted core/shell systems which compose of an AFM core and a FM or FiM shell [15–22]. Inverted nanoparticles are identified as "single-inverted" or "doubly inverted" by considering the transition temperature of core and shell parts. These unusual structures are called as "single inverted", when the Curie temperature of the FM or FiM shell is larger than the Néel temperature of the AFM core ($T_C > T_N$), such as FeO/Fe_3O_4 [23]. Doubly inverted structures are the ones with $T_N > T_C$, for instance, MnO/Mn_3O_4 [15], contrary to the conventional exchange-biased nanoparticles [17]. Doubly inverted core/shell systems have already been shown to exhibit extraordinary features, such as, non-monotonic variation of the hysteresis loop shift with core radius [15,24] and observation of exchange bias fields above T_C [22]. Moreover, inverted nanoparticles have the advantage of controlling shell structure and its magnetic properties. For instance, a new way of controlling the interface exchange coupling and hence coercivity and exchange bias is presented for inverted $CoO/Co_{1-x}Zn_xFe_2O_4$ ($x = 0 - 1$) core/shell nanoparticles very recently and it has been demonstrated that H_{ex} displays a non-monotonous behavior with Zn concentration [21].

From the theoretical point of view, the physical mechanism behind the exchange bias effects in conventional FM/AFM and FiM/AFM core/shell nanoparticles has been widely studied in literature and the origin of the exchange bias is usually attributed to the net magnetic moment pinned in AFM shell [25–28]. The effects of particle size [29–31], interfacial roughness [32], non magnetic defects [33], shape [34] and cooling field [35] on the shift in the hysteresis of conventional core/shell nanoparticles have been investigated in detail. However, except for few studies [24,36–38], less attention has been paid to the inverted nanoparticles despite the recent progress in synthesis of inverted nanoparticles.

The possibility of control of the structure of the FM or FiM shell component in the inverted nanoparticles [21] makes it interesting to address the role of microscopic parameters such as the

* Corresponding author.
E-mail address: erol.vatansever@deu.edu.tr (E. Vatansever).

https://doi.org/10.1016/j.physleta.2018.08.009
0375-9601/

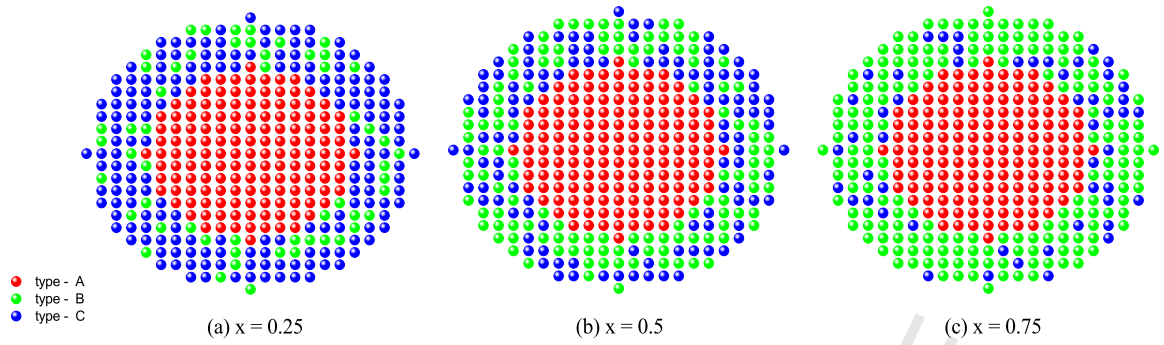

Fig. 1. Schematic representation of the two dimension cross section of nanoparticle for three selected concentration values of the type-B magnetic component, namely (a) $x = 0.25$, (b) $= 0.5$ and (c) $= 0.75$, respectively. Red, green and blue colors correspond to A, B and C types of magnetic components. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

exchange coupling between the spins of the shell, in tunning the magnetic properties of the system. In the present work, we model an inverted core/shell nanoparticle which is composed of an AFM core and a FM shell with B_xC_{1-x} which can refer to a binary alloy such as Fe_xCo_{1-x} and Ni_xFe_{1-x} by a microscopic Hamiltonian. The magnetic properties of such a system is studied by Monte Carlo simulation method based on the Metropolis algorithm. We concentrate on the dependence of coercivity and exchange bias on concentration of one of the magnetic components and exchange coupling strength between two different type of magnetic components in the shell. We have found a non-monotonic variation of both loop shift and coercivity of the system with concentration for several exchange interacting strengths which arises from the competition between different types of exchange couplings in the core and shell part of the system.

The remainder of the paper is organized as follows. In Section 2, the model of the inverted nanoparticle system is described and the details of the method used for calculation of magnetic properties of the system are presented. Our numerical results regarding the exchange bias and coercivity properties of the system are discussed in Section 3. Finally, conclusions of the work are summarized in Section 4.

2. Model and formulation

We consider an inverted nanoparticle with an AFM core and a FM shell which is obtained by cutting a sphere from a simple cubic lattice. As schematically shown in Fig. 1, the core part of the system is composed of spin-1 particles, $|\mathbf{S_i}^A| = 1$, which are labelled with A and it is coated by ferromagnetic binary alloy shell of the form B_xC_{1-x}. In order to create the binary alloy ferromagnetic shell part, we consider the spins of B and C as $|\mathbf{S_i}^B| = 1$ and $|\mathbf{S_i}^C| = 3/2$, respectively. It should be noted that $x = 1$ and 0 situations correspond to special cases where every site is filled with the B and C type magnetic components, respectively. Apart from these values of the concentrations mentioned above, the lattice sites in the shell part of the nanoparticle are randomly occupied by two different magnetic components B and C with the concentration x and $1 - x$, respectively.

The Hamiltonian of the considered system can be written in the following form:

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{\alpha\beta} \mathbf{S_i}^{\alpha} \cdot \mathbf{S_j}^{\beta} - \sum_i D_i (\mathbf{S_i}^{\alpha} \cdot \hat{\mathbf{e}}_\mathbf{i})^2 - \sum_i \mathbf{H} \cdot \mathbf{S_i}^{\alpha} \qquad (1)$$

where, α and β correspond to either of the A, B, and C magnetic components in the system and $\hat{\mathbf{e}}_\mathbf{i}$ is the unit vector in the direction of easy axis at site i. The first sum in Eq. (1) is over the nearest neighbor spins while the second and third ones are over the entire system. The spin–spin coupling $J_{\alpha\beta}$ given above can take values J_{AA}, J_{BB}, J_{BC} and J_{CC} depending on the types of the considered i.th and j.th spin pairs and it is labeled as J_{int} for the coupling of type-A and -B components and type-A and -C components at the core/shell interface which includes last layer of the core and first layer of the shell. Throughout this study, we have fixed the exchange energy constants J_{BB} and J_{CC} as unity, and the other system parameters are scaled with respect to the J_{BB}. The remaining spin–spin couplings in the shell, which correspond to the coupling between unlike magnetic components, are labelled as J_{BC} and it can take three values: $J_{BC} = 0.5J_{BB}, J_{BB}, 3J_{BB}$. If the selected spin pairs belong to the antiferromagnetic core part of the system, $J_{\alpha\beta}$ equals to $J_{AA} = -5J_{BB}$. Lastly, if the sites i and j belong to the antiferromagnetic core and ferromagnetic shell parts of the particle, i.e., at the core/shell interface $J_{int} = J_{BB}$.

Second term in the Eq. (1) refers to the magnetic anisotropy energy. D_i terms can take the values $D_c = J_{BB}$ and $D_{sh} = 5J_{BB}$ depending on the type of the selected magnetic component i in the system. If the considered spin at the position i lies in the outer layer of the shell of the particle, magnetic anisotropy is assumed to be radial. Remaining magnetic anisotropy energy contributions to the total energy of the system, except from the outer layer of the shell, are taken as uniaxial and directed along the z axis. Finally, the last summation in the Eq. (1) denotes the Zeeman term, and magnetic field is applied along the z direction. The exchange coupling and anisotropy parameters are chosen in order to simulate a doubly inverted AFM/FM core/shell nanoparticle. Namely, the Néel temperature of AFM core is larger than Curie temperature of FM shell ($T_N > T_C$) for all the considered x values ($0 \leq x \leq 1$), namely the nanoparticle is doubly inverted. It should be noted that tuning the alloy concentration in the shell also may cause to variation in the magnetic anisotropy strengths, effective anisotropy axis and also crystal structure of the shell. However, for simplicity, we neglect these effects throughout the work.

We implement Monte Carlo simulation with local spin update Metropolis algorithm [39,40] to investigate magnetic properties of the present system. Throughout this study, we select the core and shell thickness as $t_c = 7a$ and $t_{sh} = 4a$ such that total radius of the particle is $t = t_c + t_{sh} = 11a$, which are expressed in lattice spacings. We use free boundary conditions which allow us to consider the finite size of the nanoparticle. We can briefly summarize the simulation procedure followed in this work as follows. We have simulated 20–40 disorder realizations to collect the data for thermal variations of magnetization curves as well as magnetic hysteresis curves for each selected values of the concentration, x. In each sample realization, the Monte Carlo simulation starts at the high temperature regions, then the temperature is slowly decreased until the desired temperature, $k_BT/J_{BB} = 0.01$, is reached in the presence of cooling magnetic field of $H/J_{BB} = 4$. The last spin configuration obtained for the desired temperature is used as initial spin configuration for the decreasing branch of

Please cite this article in press as: Z.D. Vatansever, E. Vatansever, Tunning exchange bias in inverted antiferromagnetic/ferromagnetic core/shell nanoparticles by binary alloy shells, Phys. Lett. A (2018), https://doi.org/10.1016/j.physleta.2018.08.009