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Exchange bias for core/shell magnetic nanoparticles

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ABSTRACT

We study the properties of a finite magnetic system to model a magnetic nanoparticle, which is formed by a reduced number of magnetic dipole moments due to the spin of the atoms. The nanoparticle is of the type core/shell where the shell is formed by spins interacting through an antiferromagnetic exchange coupling while for the spins belonging to the core the coupling is ferromagnetic. The interaction between the spins at the interface core/shell can be either ferro or antiferromagnetic. To describe the states of the spins we used the XY model in which the spins are considered as continuous variables, free to point in any direction of the xy plane. We also consider a magnetocrystalline anisotropy, exchange anisotropy and the Zeeman effect. Our model is studied in a lattice with square symmetry, using the Monte Carlo method along with the Metropolis prescription. The results show that in the absence of an external magnetic field and exchange anisotropy, the system continuously goes to a disordered state from an ordered state at a well defined temperature. In the presence of external magnetic fields the system displays the exchange bias phenomenon, that is, the displacement of the hysteresis loops, due to the introduction of the exchange anisotropy term. However, this displacement depends on the core and shell sizes, as well as on the magnitude of the coupling between the shell and the core moments.

1. Introduction

The magnetic properties of materials are so rich and interesting that, even after many years, the study of magnetic systems is able to surprise us. In fact, since ancient Greece, when the phenomenon of attraction and repulsion of magnetic stones was revealed [1] and besides all scientific knowledge built over the years, we are constantly faced with new discoveries, mainly after the sixties, in which news techniques for production of magnetic nanoscopic samples were developed. For instance, we can cite superparamagnetism [2,3], magnetoresistance [4], giant magnetic resistance [5] and exchange bias [6]. In general, these new phenomena occur in nanoscopic scale and, therefore, are known as nanomagnetic ones. To understand these phenomena we can use experimental techniques, analytical approaches or computational simulations [7–9].

Among the interesting phenomena, the exchange bias is related to the shift of the hysteresis loop in magnetic systems in which there is an interface between two different kinds of magnetic materials, like in multilayer thin films and magnetic nanoparticles of core/shell type [10,11]. In order to observe the exchange bias, magnetic samples at high temperature must be cooled below the Neél (T_N) and Curie (T_C) temperatures, in the presence of an external magnetic field (FC: field cooling). If this magnetic field is zero (ZFC: zero field cooling) the displacement of the hysteresis loop does not occur.

In order to understand this phenomenon in more detail consider an interface between two different magnetic layers. In one of them (FM) the magnetic dipoles interact through a ferromagnetic coupling and in the other (AFM) the exchange interaction is antiferromagnetic. The exchange interaction between spins on different layers is ferromagnetic. The order–disorder

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transition temperature for the two layers is T_C (FM) and T_N (AFM) such that $T_C > T_N$. If the temperature of the system is larger than T_C, both layers are disordered and the hysteresis loop is not observed. When the system is cooled to a temperature ($T_N < T < T_C$) the normal hysteresis loop appears for the ZFC and FC processes. But when the system is put in a temperature less than T_N, we experimentally observe a difference between the FC process and the ZFC one. In fact, when the system is cooled in a ZFC process the resultant hysteresis loop is normal. Surprisingly, in the FC process all the hysteresis curves undergo a displacement, in general to the left, modifying the values of the coercive fields relative to the values obtained in the other procedures [12–17].

The first work that showed this phenomenon was performed by Meiklejohn and Bean [6] at fifties. They used *Co/CoO* particles with a core/shell structure where the spins of the core did interact through a ferromagnetic coupling while the spins of the shell did interact through an antiferromagnetic coupling. To explain the hysteresis loop displacement, the authors argued about a new kind of anisotropy (now called exchange anisotropy) able to make the magnetic dipole moments on the interface between core and shell to point to a privileged direction and, so, breaking the symmetry of the hysteresis curves.

Despite recent experimental works on this subject considering different magnetic materials [12–22], analytical approaches and computational simulations are needed to better understand it [22–32]. Therefore, in this work we propose a model to study the magnetic behaviour of a core/shell magnetic nanoparticle formed by a finite number of magnetic moments, which are due to the atomic spins of the atoms. The spins can continuously change direction in the *xy* plane and the interaction between a pair of spins is short-ranged [33]. Due to the fact the spin variables are continuous we choose a two dimensional lattice, instead of a three dimensional one, because the exchange bias phenomenon is already observed in low dimensions and also the computational calculations are less expensive. In our model, the exchange interaction between spins belonging to the core is ferromagnetic while it is antiferromagnetic between the spins belonging to the shell. The interaction between spins located at the interface core/shell can be ferromagnetic or antiferromagnetic. Besides, we take into account the spin–orbit interaction, considering a magnetocrystalline anisotropy term, and the Zeeman effect.

In order to better understand the exchange bias we also consider the anisotropic term introduced by Meiklejohn and Bean [6]. The main features of this term are: (a) to make the spins vectors to point in the same direction of the external magnetic field in a FC process and (b) to act only on the spins of the interface located in the shell subsystem.

The magnetic quantities associated with the model are obtained using the Monte Carlo simulation with Metropolis prescription [34]. Our results show that the displacement of the hysteresis loop occurs only if the term of exchange anisotropy is included into the model. However, all results are strongly dependent on the parameters of the model.

The simulation of nanoparticles in lattices is the simplest way to get information relative to the assembly of large magnetic moments at finite temperatures. The Landau–Lifschitz–Gilbert equation that describes the dynamics of the magnetization vector in continuous systems is limited to the very small time scales. However, if one intends to investigate the magnetic properties of an assembly of nanoparticles for a long time, the best way is to consider lattice models along with Monte Carlo simulations. For instance, very recently interesting problems related to the role of dipolar interaction in magnetic hyperthermia [35,36] and the competition between cubic and uniaxial anisotropies in the study of relaxation in magnetic experiments [37,38] have been investigated in lattices along with Monte Carlo simulations.

Our work is structured in such way that in Section 2 we introduce the model for the core/shell magnetic nanoparticle and the numerical simulation procedures. In Section 3 we show and discuss the results and finally, in Section 4, we present our conclusions.

2. Model and Monte Carlo simulation

The magnetic nanoparticle considered in this work consists in a *XY* model on a two dimensional square lattice of spins, which can continuously point to any direction in *xy* plane. The particle, as shown in Fig. 1, is composed by two regions: (a) a core, in which the exchange interaction between first neighbours spins is ferromagnetic and (b) a shell involving the core composed by spins whose exchange interaction between first neighbours is antiferromagnetic. The coupling core/shell is given by an exchange interaction between the spins located at last layer of the core with the spins at the first layer of the shell.

In order to ensure a privileged direction for the particle magnetization (easy axis) we consider a magnetocrystalline anisotropy term pointing in the *x* direction, which is the same for all the spins belonging to the particle. The external magnetic field necessary to construct the hysteresis curves can point to any direction in the *xy* plane.

Taking into account the previous definitions, the Hamiltonian of our model is given by

$$\mathcal{H} = -\sum_{i,j} J_{ij}\vec{\sigma}_i \cdot \vec{\sigma}_j - D\sum_i (\vec{\sigma}_i \cdot \vec{e}_x)^2 - \sum_i \vec{H} \cdot \vec{\sigma}_i, \tag{1}$$

where J_{ij} is the magnitude of the exchange interaction between the spins $\vec{\sigma}_i$ and $\vec{\sigma}_j$. It is positive ($J_{ij} = J_c > 0$) in the core and negative ($J_{ij} = J_s < 0$) in the shell. At the interface $J_{ij} = J_i$ can be positive or negative, but non null. Here, we choose J_i as a positive quantity by reasons that will be clear in the next section. The double sum in the first term occurs only between first neighbour pairs of spins, considering the different forms of interaction, while the sum in the second and third terms are over all the spins of the lattice. The spin variables can be written as a function of their components along the *x* and *y* directions by $\vec{\sigma} = \sigma_x\vec{i} + \sigma_y\vec{j}$ with $\sigma_x = \cos(\theta)$ and $\sigma_y = \mathrm{sen}(\theta)$, in which the angle θ is measured with respect to the *x* axis taking into account $|\vec{\sigma}| = 1$. The magnetocrystalline anisotropy defines the easy magnetization axis $\vec{e}_x$, chosen to point along the *x* direction with magnitude D. Finally, $\vec{H}$ represents the uniform external magnetic field.