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ScienceDirect
Physica B 403 (2008) 390–393
PHYSICA B
www.elsevier.com/locate/physb

Monte Carlo simulation of Fe–Co amorphous nanoparticles magnetization

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Abstract

Magnetization simulations of ~3 nm non-interacting Fe–Co ferromagnetic amorphous nanoparticles were made using Metropolis algorithm of Monte Carlo method. The results of core–shell model simulations describe the nanoparticles as a ferromagnetically ordered core and a disordered surface shell. They fairly reproduce the significant features observed in 3 nm Fe–Co–B nanoparticles experimental magnetization measurement at the same Fe–Co composition. They also provide a clear evidence of the role played by the local surface anisotropy and the surface–core exchange interaction in determining the magnetic properties of the nanoparticles.

PACS: 75.50.Tt; 75.40.Mg; 75.75.+a; 75.60.Jk

Keywords: Ferromagnetic nanoparticles; Surface effects; Monte Carlo simulation; Magnetization measurements

1. Introduction

Finite-size effects dominate the magnetic properties of nanosized particles, due to the increasing surface-to-volume ratio. Surface effects basically result from the surface anisotropy presence, commonly uniaxial, which lead to surface spin misalignment with respect to the ordered core spins. This effect has been reported in magnetization measurements of Fe–Ni–B and Co–Ni–B amorphous nanoparticles [1,2], γ-Fe_2O_3 nanoparticles [3], NiO nanoparticles [4], and simulated by Monte Carlo (MC) calculations [3,5–7].

In a previous work [7], we have presented a Metropolis algorithm for simulating the ferromagnetic amorphous nanoparticles magnetization in both superparamagnetic and blocked regimes. In this case, the surface anisotropy, which depends on the surface topology, competes with the exchange interaction leading to surface spin misalignment with respect to the ordered core spin. At low temperatures, ferromagnetically ordered regions grow in the surface and interact between them and the core giving cluster-glass behavior. In the case of Fe–Co–B nanoparticles, the effect of different easy axis on surface anisotropy should be added to this magnetic frustration. The iron surface anisotropy is perpendicular to the surface while the cobalt surface spins have the easy axis direction parallel to the surface. Then, an unusual magnetic behavior is expectable in nanoparticles with approximately the same amount of Co and Fe in the composition.

On the other hand, Fe–Co–B nanoparticles have particular interest because the atomic magnetic moment of the Fe_xCo_{1-x} alloys shows variation with composition following the known Slater–Pauling curve, which presents a maximum at $x = 0.65$ with a magnetic moment $\mu \approx 2.45\mu_B$ per atom (~240 emu/g) [8]. This magnetization is larger than pure metallic Fe or Co.

In this context, amorphous ferromagnetic particles deserve a special attention because of the intrinsic structural disorder in both particle core and surface. We present the results of magnetization measurements of 3 nm $(Fe_xCo_{1-x})_{60}B_{40}$ amorphous nanoparticles and we explain

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doi:10.1016/j.physb.2007.08.057

the experimental results with Metropolis algorithm in the MC simulations, which satisfactorily reproduce the magnetization vs. temperature curves observed experimentally.

2. Experimental results

Magnetization measurements on ~3 nm $(Fe_xCo_{1-x})_{60}B_{40}$ amorphous nanoparticles were performed as a function of temperature ($5\,K < T < 300\,K$). These particles have been previously described in Ref. [9] and are dispersed in a polymer (polyvinyl–pyrrolidone) to prevent interparticle interaction with an estimated mean center-to-center interparticle distance $d = 35$ nm. The interparticle distance is so large that dipole–dipole interactions are negligible. The magnetization measurements performed according to the standard zero-field-cooling (ZFC) and field-cooling (FC) procedures show for all the samples magnetic irreversibility between FC and ZFC curves up to room temperature, revealing a high effective anisotropy energy barrier (Fig. 1). The observed behavior shows the progressive blocking of nanoparticles moments, with a distribution of the anisotropy energy barriers. With decreasing temperature, surface spin fluctuations slow down and short-range interactions between surface spins develop, resulting in a progressive formation of regions of magnetically correlated spins of growing size that finally give rise to a frozen, disordered surface–spin state (likely a cluster-glass state), responsible for the growing of the magnetization of the $Co_{60}B_{40}$ nanoparticles at low temperatures (Fig. 1a). This low temperature behavior is not observed in $Fe_{60}B_{40}$ nanoparticles, as is shown in Fig. 1b.

On the other hand, $(Fe_{0.69}Co_{0.31})_{60}B_{40}$ nanoparticles present anomalous magnetic behavior. As it is shown in Fig. 1c, the FC magnetization of these nanoparticles decreases as the temperature is decreased. This behavior is unexpected in non-interacting single-domain systems at the blocked regime. In this case, the FC magnetization increases when temperature decreases and in the interacting nanoparticles the FC magnetization remains constant or is slightly reduced when temperature decreases. In our case, the intraparticle interactions (i.e., the interaction between the magnetically ordered regions in the surface with the ordered core of the particle) would be the responsible of the observed behavior. These nanoparticles also present an increasing of the magnetization at low temperatures.

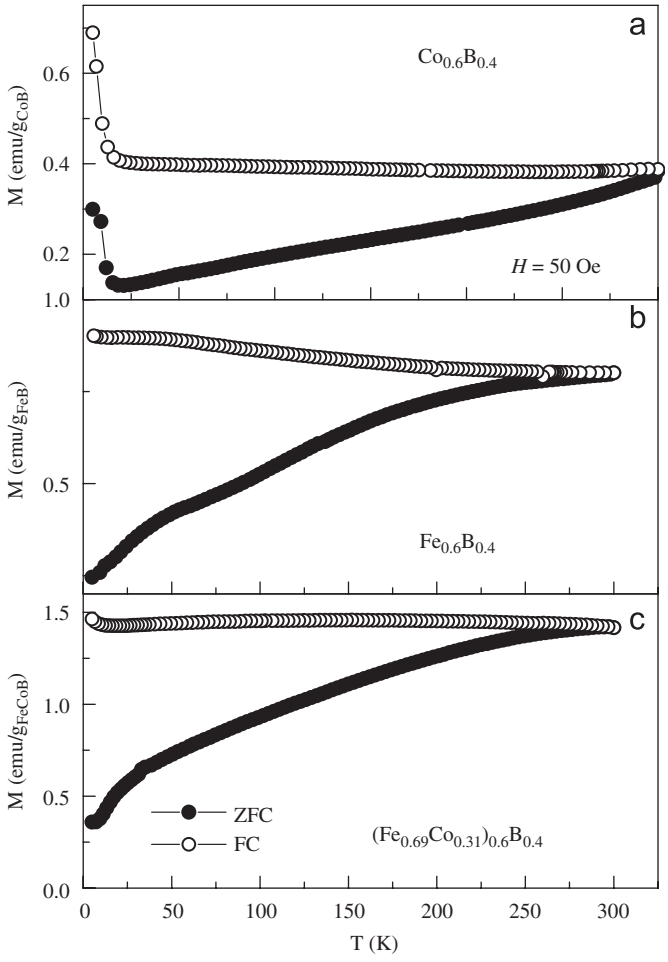

Fig. 1. $M(T)$ curves measured under zero-field-cooling (solid circles) and field-cooling (open circles) conditions at $H = 50$ Oe for ~3 nm $Co_{60}B_{40}$ (a), $Fe_{60}B_{40}$ (b), and $(Fe_{0.69}Co_{0.31})_{60}B_{40}$ (c) amorphous nanoparticles.

3. Monte Carlo simulation results and discussion

We consider a model in which the particles are composed by a magnetically ordered core containing N_{core} spins and a disordered shell surrounding it, containing N_{shell} spins of magnetic moment μ_i (μ_i is the magnetic moment of Fe or Co depending of the composition). The total energy per particle is given by [1,2,7]

$$E = -K_{core}(\hat{\boldsymbol{\mu}}_{core}\cdot\hat{z})^2 - \boldsymbol{\mu}_{core}\cdot\mathbf{H} - \sum_{\langle i,a\rangle}^{N_{shell}} J_{i,a}^{shell}\mathbf{S}_i\cdot\mathbf{S}_{i+a} - \sum_{i}^{N_{surf}} K_i^{surf}(\hat{\mathbf{S}}_i\cdot\hat{\mathbf{n}}_i)^2 - \sum_{i}^{N_{shell}}\boldsymbol{\mu}_i\cdot\mathbf{H}, \quad (1)$$

where μ_{core} and K_{core} are the core magnetic moment and anisotropy constant, respectively, $J_{i,a}^{shell}$ is the exchange constant per ion between shell–shell ions and core spins–shell ions interaction (Co–Co, Fe–Fe or Co–Fe), K_i^{surf} is the surface anisotropy per atom (Fe or Co), and $\hat{\mathbf{n}}_i$ indicates a unit vector perpendicular to the surface. The surface anisotropy term tends to align the spins perpendicular (parallel) to the surface for Fe (Co) magnetic moment, as reported in the literature [7]. The anisotropy terms determine an energy diagram with two minima separated by an energy barrier, which is modified by the applied magnetic field. Depending on the temperature and the energy barrier, the system will be in superparamagnetic regime (thermal-equilibrium) or in the blocked regime (non-equilibrium or metastable state).

The implementation of the MC simulation based on Metropolis algorithm on this problem minimizes the system internal energy (defined by Eq. (1)) by randomly varying the