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Effect of the Sign of Anisotropy Constants on the Properties of the System of Interacting Ferromagnetic Nanoparticles

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We use the Monte Carlo simulation method to investigate the influence of the signs of magnetocrystalline anisotropy constants and the magnetic dipole–dipole interactions on the zero field cooled–field cooled magnetization experiments and hysteresis curves of a system of magnetic nanoparticles. Positive first cubic anisotropy constant K_1 results in larger blocking temperatures and larger coercive fields of a system, while the second anisotropy constant K_2 is practically of negligible importance for the phenomena investigated. Magnetic dipole–dipole interactions are important only in the most dense systems of particles and their effects practically disappear for systems where the distance between the closest particles exceeds three particle diameters.

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1. Introduction

Much experimental and theoretical effort is recently being devoted to understand magnetic properties of systems of magnetic nanoparticles embedded in an otherwise nonmagnetic material. Such systems occur in attempts aiming at creating ferromagnetic semiconductors — typically of III–V groups: GaAs:Mn or GaN:Mn and GaN:Fe with the concentration of magnetic ions high enough to approach room temperature ferromagnetism. These attempts usually result in the formation of ferromagnetic precipitations. Thermal annealing applied to $Ga_{1-x}Mn_xAs$ layers leads to formation of MnAs dots, similarly, in metal-organic vapor phase epitaxy (MOVPE)-grown (Ga,Fe)N ferromagnetic FeN_x nanocrystals aggregate by precipitations [1–3]. Such mixed systems of ferromagnetic grains in a semiconductor host are often called nanocomposites and are potentially promising candidates for information storage and spin electronics applications [3]. Ferromagnetic particles embedded in non-magnetic environments are also of much interest in geology [4]. Such inhomogeneous systems cannot yet be modeled within the *ab initio* methods and one must rely on more phenomenological approach to account for a large variety of physical effects that determine system's properties. For instance, when modeling ferromagnetic (or superparamagnetic) properties it is necessary to include magnetocrystalline anisotropy of single-crystal domains within each ferromagnetic nanoparticle as well as its interaction with external magnetic field and other nanoparticles randomly distributed in space. Here we apply the Monte Carlo method to study magnetic properties of an ensemble of randomly oriented, spherical, single-domain ferromagnetic nanoparticles with cubic anisotropy. To be as close as possible to real systems, in addition to magnetic anisotropy our model includes also the dipole–dipole interparticle interactions, the effects of particle volume and inter-particle distances. We simulate zero-field cooled–field cooled (ZFC/FC) experiments and calculate hysteresis curves.

2. The investigated system

As our theoretical model we investigate a disordered system of 27 single-domain (single-crystal) ferromagnetic particles. Each particle is treated as one magnetic dipole located in particle's center and of constant magnetic moment equal to the moment of a homogeneous, bulk fcc crystal of the same volume — that is no surface anisotropy is included. Positions of particles and orientations of their crystallographic axes are chosen randomly and are fixed within the calculations. In most densely packed systems considered particles' positions are chosen in such a way that the surface of each particle touches the surface of at least one other nanoparticle. To investigate the role of packing-density of particles we compare results of calculations in which all distances between the particles are multiplied by the scaling factor (sf) with sf = 1 for the most dense systems and sf = 8 for the most diluted one. Absolute values of the cubic magnetocrystalline anisotropy constants are taken equal to the ones for bulk fcc cobalt, for which, close to $T = 0$ K, values $K_1 = -2.7 \times 10^6$ erg/cm^3 [4] and $K_2 = -2.0 \times 10^5$ erg/cm^3 [5, 6] are to be found in the literature. We compare results for all four possible combinations of signs of K_1 and K_2.

3. Computational procedure

Monte Carlo simulations were carried out using the standard Metropolis algorithm [7] applied to a cluster of 27 randomly distributed Co nanoparticles. The model Hamiltonian of the system includes the cubic magnetocrystalline anisotropy energy, the energy of dipole–dipole interactions between particles and the term representing the interaction of each magnetic moment with an external field B:

$$E = \sum_i E_{\text{anis}}(\boldsymbol{m}_i) + \sum_i E_{\text{dip-dip}}(\boldsymbol{m}_i, \boldsymbol{m}_j) + \boldsymbol{B}\sum_i \boldsymbol{m}_i.$$

Magnetic moments m_i are allowed only to rotate in a fixed place in space. 10 000 Monte Carlo steps (MC steps) of thermalization are followed by 10 000 MC steps to collect the data. The results are then averaged over 10 independent MC cycles and additionally averaged over 20 such MC runs for different configurations of nanoparticles. FC and ZFC curves (in the temperature range of 2–400 K) as well as hysteresis loops (with magnetic field cycled from −6 T to +6 T) are calculated for particles of 6 nm in diameter and concentrations from sf = 1 to sf = 8 to investigate the influence of the density of the system on the blocking temperature T_b and the coercive field B_c of the sample. Our previous work was related to negative anisotropy constants [8, 9]. To investigate the role of the sign of anisotropy constant calculations were repeated for the same absolute values of the magnetocrystalline anisotropy constants K_1 and K_2 and different combinations of their signs (+ +), (+ −), (− +), and (− −).

4. Results and discussion

In Figs. 1 and 2 we present results of our simulations of ZFC/FC experiments for particles of 6 nm in diameter for three different sf values: sf = 1, 2, and 8. In each simulation, first, our sample is cooled with no magnetic field to the temperature $T = 2$ K, then the external magnetic field $B = 0.01$ T is switched on and temperature is raised in steps of 1 K from $T = 2$ K to 400 K. Subsequently our sample is cooled from 400 K to 2 K with the magnetic field kept at its constant value $B = 0.01$ T. The whole simulation is then repeated for all four combinations of signs of constants K_1 and K_2. In all cases positive K_1 value results in considerably larger blocking temperatures T_b and smaller magnetization after field-cooling than in the case of $K_1 < 0$. With increasing sf the role of dipole–dipole interactions diminishes which results in increased values of FC magnetization at low temperatures. As seen in Figs. 1–3 the sign of the K_2 anisotropy constant (for the realistic values taken as for fcc Co) is practically of no effect on the ZFC/FC experiments with practically indiscernible curves for the same K_1 values and opposite signs of K_2.

Figure 2a–c presents our results for hysteresis curves for the same systems of 27 nanoparticles at $T = 2$ K and for scaling factors sf = 1, 2, and 8. Hysteresis curves for $K_1 > 0$ are much broader — i.e. coercive fields B_c are much larger — than for $K_1 < 0$. Strong dipole–dipole interactions in most densely packed systems (sf = 1) result in thin, inclined hysteresis curves. Although the overall shapes of hysteresis curves for sf = 2 and 8 are very similar the latter ones have sharper (less rounded) "corners" as the sign of weak interactions between magnetic mo-

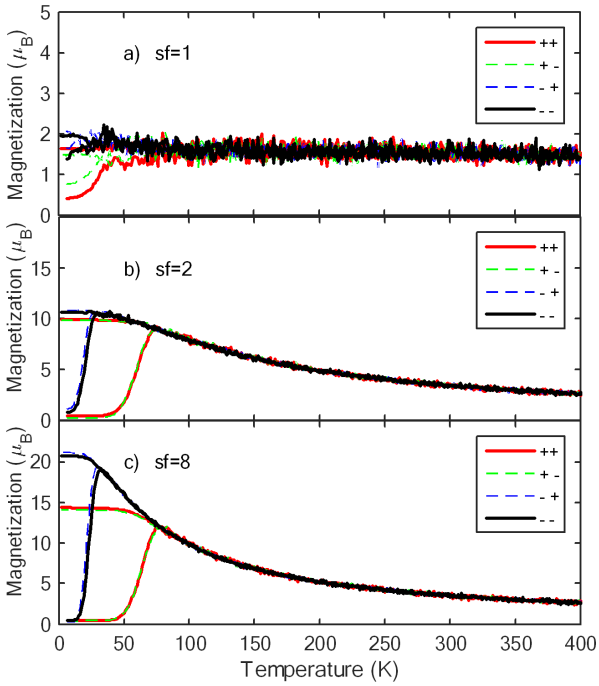

Fig. 1. ZFC-FC curves at 0.01 T for different sign of (K_1, K_2) and different scaling factors (a) sf = 1, (b) sf = 2, (c) sf = 8.

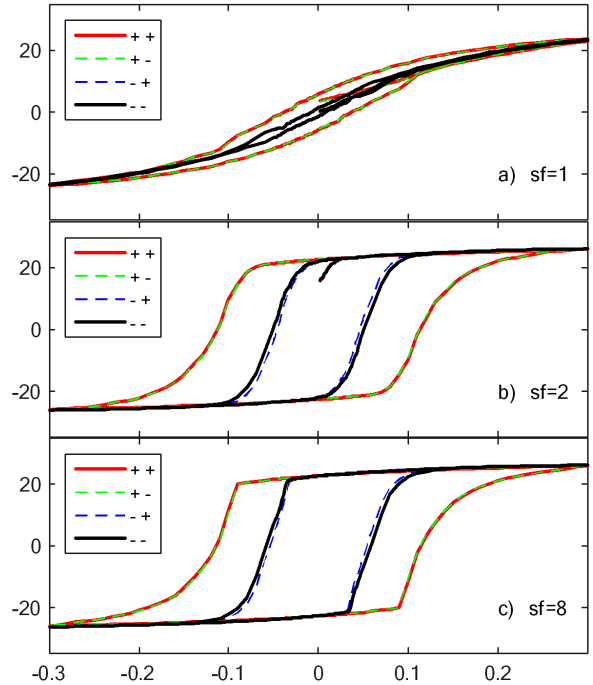

Fig. 2. Hysteresis loops at 2.0 K for different sign of (K_1, K_2) and different scaling factors (a) sf = 1, (b) sf = 2, (c) sf = 8.

ments still present in the system. Again, changing the sign of K_2 leads to only hardly visible changes in the shapes of corresponding hysteresis curves.

5. Summary

In this short report we present results of our simulations of magnetic properties of a cluster of ferromagnetic nanoparticles embedded in a nonmagnetic host. We investigate the role of the signs of magnetocrystalline anisotropy constants and the influence of magnetic dipole–dipole interactions on the ZFC/FC magnetization experiments and hysteresis curves. We conlcude that positive first cubic anisotropy constant results in larger blocking temperatures and larger coercive fields of a system, while the second anisotropy constant is practically of negligible importance for the phenomena investigated. Magnetic dipole–dipole interactions are important only in the densest systems of particles and their effects practically disappear for sf > 3.

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