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#### HYSTERESIS PROPERTIES OF TWO-DIMENSIONAL SPIN SYSTEMS

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We present the numerical results of the temperature, the core radius, and the exchange interaction constant influence on the coercitivity and the exchange bias field of the core-shell spin system. We clarified, that the coercitivity disappeared and the exchange bias reduced with the temperature. It is shown, that the coercitivity grows with the core radius. At the same time, the exchange bias field shows the nonuniform dependence, because it is a function of outer layer type. When the constant of the exchange bias field increases as well, but the coercitivity decreases.

*Keywords:* TWO-DIMENSIONAL SPIN SYSTEMS, CORE-SHELL PARTICLE, COERCITIVITY, EXCHANGE BIAS FIELD, MAGNETIC HYSTERESIS.

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#### **1. INTRODUCTION**

Studying the properties of magnetic nanoobjects is a top-priority task in a modern science. This is caused by an extensive application field of such objects, for example, for information recording [1], magnetic-field sensors [2], strong permanent magnets, ferrofluid production [3] and others. Yearning for deeper understanding the processes of magnetism at nanolevel is the motivation for their studying as well.

Magnetoresistive random-access memory (MRAM) [2, 4] is one of the instances of magnetic nanoparticles application in IT-industry. It is the most promising type of nonvolatile memory (NVRAM), which uses the magnetic moment direction for information storage. A cell of such memory is a magnetic nanoparticle with a complex structure. It consists of the fixed magnetic layer (uniform ferromagnetic area with constant magnetization), the tunnel magnetic transition, and the free magnetic layer (uniform ferromagnetic area with magnetization depending on the external magnetic field action). The tunnel magnetic transition is a thin dielectric layer. The electrical resistance of a cell strongly depends on the mutual magnetizations orientation in the free and the fixed layers. This is the result of the effect of tunnel magnetoresistance (see, for example, [5]). So, measuring the electrical resistance of such a cell, the information read-out can be performed. Rerecording is realized by the magnetic moment reversal of the free layer [6].

Another important, from the practical point of view, example of magnetic nanoparticles is the complex particles, which consist of the ferromagnetic (FM) core and the antiferromagnetic (AFM) shell. Such particles application allows to solve one of the problems, which are the result of IT-devices miniaturization and connected with this the decrease of particles size, namely, rising influence of thermal fluctuations on magnetic

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moment [7, 8]. One of the methods of such structures production is an oxidation of the fine ferromagnetic particles. When they are in an oxygencontaining medium they are easily covered with an oxide layer, which is an antiferromagnetic. For the prevention of their total oxidation the medium with controllable oxygen content [9] is used.

The ensembles of such nanoparticles have great prospects of application in so-called magnetic storages with perpendicular recording, work surface of which represents a texture (perpendicular patterned media or bit-patterned media) [10, 11]. Nowadays in widespread hard disks information is coding by the certain direction of domains magnetization, lying in the working surface plane. In contrast to this in mentioned devices every information bit will connect with one particle only, the magnetization moment of which can be directed in one of two directions only, perpendicular to the particles distribution plane. This allows to considerably raise the data density. At present there are hard disks with perpendicular data recording. Thus, the famous company Hitachi not long ago has started production of devices with 1 Tbyte capacity [12]. The predicted recording density of storage devices with perpendicular recording is ~ 100 Tbyte/inch<sup>2</sup>.

In particles with complex structure of the core-shell type the unidirectional anisotropy [13] takes place, which is the result of interaction between spins of the FM core and the AFM shell. The longitudinal displacement of a hysteresis loop, describing the behavior of complex magnetic nanoparticles in external field, is one of displays of such interaction. This displacement is called as the exchange bias one.

In spite of the exchange bias phenomenon was discovered more than 50 years ago [14], its intensive studying is carrying out currently, what is connected with development and upgrading of magnetic nanoparticles production technology. Along with the experimental study [7] the numerical simulation [15-23], based on the Monte-Carlo methods [24, 25], has a wide-spread occurrence.

# 2. MODEL AND BASIC EQUATIONS

For simulation the magnetic properties of a complex nanoparticle each its atom is assigned the magnetic moment vector  $\mathbf{S}_i$ , which has a constant magnitude, and its direction is giving by a continuous set of the polar angle values  $\varphi \in (0; 2\pi)$ . Such magnetic moments are called as the spin ones and are situated in the lattice sites. Taking into account the limited simulation possibilities we study the two-dimensional square lattice only.

Let us consider a part of such lattice bounded by a circle with the radius  $R + \Delta R$ . Vectors  $\mathbf{S}_i$  interact with each other via exchange interaction. Interaction inside a circle of the radius R is the ferromagnetic one and characterized by the constant of exchange interaction  $J_C$ , and inside a ring with the internal radius R and the thickness  $\Delta R$  the interaction is the anti-ferromagnetic one with the constant  $J_S$ . Interaction of the core interface spins is characterized by the constant  $J_{If}$ .

For such a system we wrote the Hamiltonian, reduced to the Boltzman constant [20, 27]

$$\frac{H}{k_B} = -J_C \sum_{\langle i,j \in C \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - K_C \sum_{i \in C} \left( \mathbf{S}_i \cdot \mathbf{e}_i \right)^2 - J_S \sum_{\langle i,j \in C \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - K_S \sum_{i \in S} \left( \mathbf{S}_i \cdot \mathbf{e}_i \right)^2 - J_{If} \sum_{\langle i \in C, j \in S \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \mathbf{h} \cdot \sum_i \mathbf{S}_i ,$$
(1)

where H is the total system energy;  $k_B$  is the Boltzman constant;  $K_C$  and  $K_S$  are the anisotropy constants of the core and the shell, respectively; **h** is the external magnetic field. Summation in the first, the second and the third terms of expression (1) is performed for magnetic moments of the FM core, in the forth term – for magnetic moments of the AFM shell, in the fifth term – over the interface magnetic moments, in the sixth term – over the all spins of a particle. The angle brackets denote the summation over the nearest neighbors.

Consider the case, when the easy magnetization axis of the core coincides with the similar shell axis. Assume, that the core anisotropy constant  $K_C$  is much larger than the shell anisotropy constant  $K_S$  what is typical for cobalt particles, covered by an oxide layer [14]. In this case the mechanism of the exchange bias field  $H_{EB}$  appearance is following. Under the external alternating magnetic field  $\mathbf{h}(t)$  action on a particle, the core spin magnetic moments undergo its orientation action, while the shell spin moments are keeping by a stronger effective anisotropy field. Shell spin magnetic moments, which directly border upon the FM core due to interaction through the interface ferromagnetic/antiferromagnetic, condition the certain preferred direction of the core spin magnetic moments. This is equivalent to the action of some effective constant field, which is called as the exchange bias one [26]. Such a field appears in the hysteresis loop shifting (see Fig. 1).

Presented in Fig. 1 results are obtained within the Heisenberg model realization for the following parameters: R = 9d, where d is the lattice spacing;  $\Delta R = 2d$ ;  $J_C = 5$  K;  $J_S = -5$  K;  $J_{If} = -2.5$  K;  $K_C = 1$  K; T = 0.1 K. An external field was applied along the easy magnetization axis and was changing in the



**Fig. 1** – Simulation results of magnetic hysteresis of a coated nanoparticle (the Heisenberg model): for fixed shell spins (1), for field-cooled particle (2), for the case of an absence of interaction in the particle interface layer (3)

range  $h \in [-15; 15]$  K with the step  $\Delta h = 0,1$  K. The number of Monte-Carlo steps for every field value is  $N = 5 \cdot 10^3$  per spin. The reduced magnetization of the FM core corresponds to the vertical axis of Fig. 1 and was calculated as follows:

$$M = \frac{1}{N_R} \left| \sum_{i \in R} \mathbf{S}_i / S \right|, \qquad (2)$$

where  $N_R$  is the number of spin magnetic moments of the core;  $S = |S_i|$ .

The exchange bias field  $H_{EB}$  and the coercitivity  $H_C$  are determined from Fig. 1 as

$$H_{EB} = (H_{cl} + H_{cr})/2, \ H_C = (H_{cr} - H_{cl})/2.$$
(3)

Two simulation models of the spin systems- the Ising model and the Heisenberg one – were considered in the paper [26], and it was shown that the Heisenberg model gives more reasonable results. That is why we use just this model in the present work.

# 3. EXCHANGE BIAS FIELD DEPENDENCE ON DIFFERENT SYSTEM PARAMETERS

#### **3.1 Temperature dependences**

Behavior of the exchange bias field and the coercive one with changing the system parameters is of natural interest. This interest is dictated by the practical reasons: it is possible to take an advantage of a new property, only having the in-depth information about all its features. And temperature is one of the most important system parameters.

With temperature rise any magnetic ordering will be destructed. On the assumption that the FM core anisotropy is less, than the AFM shell one, for simulation simplicity we suppose that the shell spins do not undergo the thermal fluctuations and have the fixed-given antiferromagnetic ordering.

Simulation result within the above-mentioned assumption is presented in Fig. 2. Here the simulation parameters are the following: R = 9d,  $\Delta R = 2d$ ;  $J_C = 10$  K;  $J_{If} = -5$  K;  $K_C = 1$  K. An external field was applying along the easy magnetization axis and was changing in the range  $h \in [-3,5;3,5]$  K with the step  $\Delta h = 0,1$  K. The number of Monte-Carlo steps for every field value is  $N = 1 \cdot 10^3$  per spin. Decrease of the curve (1) to zero denotes the destruction of the core ferromagnetic ordering. As a result there is the week decay of the exchange bias field as well, since the bond between fixed shell and core spins becomes less significant in fluctuating dynamics of the core spin moments.

#### **3.2 Dependences on the core radius**

Since the unidirectional anisotropy is the result of a number of surface effects, it should demonstrate the essential dependence on geometric parameters of nanoparticle. In our case a particle has the round form and the core-shell interface geometry will depend on the particle radius by two reasons. The first reason is the specific energy contribution of the interface interaction in comparison with the total energy. The interaction energy of the spin magnetic moments in the core is proportional to a number of moments, which, by-turn, depends on the radius R by the quadratic law. At the same time, increase of the radius R leads to a linear growth of the surface spin magnetic moments. That is why the investigated effect will be pronounced for comparatively small particles. The second reason consists in different form of the interface layer, and the R variation per unit can lead to significant structural changes of the surface layer and, later on, of the particle reversal process nature.



Fig. 2 – Temperature dependences of the coercitivity  $H_C(1)$  and the exchange bias field  $H_{EB}(2)$ 

The first step of the unidirectional anisotropy investigation for different sized particles is finding the  $H_C(R)$  and  $H_{EB}(R)$  dependences, as in the case of the temperature dependence, for the fixed spin magnetic moments of the shell (see Fig. 3). Here the simulation parameters are the same as in the previous case but with another temperature T = 0.1 K, and the number of Monte-Carlo steps for every field value is  $N = 2 \cdot 10^3$  per spin.



Fig. 3 – Dependences of the coercitivity  $H_C(1)$  and the exchange bias field  $H_{EB}(2)$  versus the particle radius

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As seen from Fig. 3, the coercitivity  $H_C$  increases with the radius due to the growth of magnetic energy of the core spin magnetic moments. At the same time, as it was expected, the exchange bias field  $H_{EB}$  shows the non-monotonic dependence at large values of the radius R. In Fig. 4 we present two different types of the surface layer formation, which condition different influence degree of the surface effects and, therefore, different values of the  $H_{EB}$ . Particles with the core radius 5, 6, and 9 have the same structure as in Fig. 4a, so, the bias field values are lager for them than for particles with another radius.



Fig. 4 – Different types of the interface layers: R = 7d (a); R = 8d (b)

The more realistic situation, when the shell spins are under thermal fluctuations as well, shows the qualitatively similar dependences  $H_C(R)$  and  $H_{EB}(R)$ . We have done the series of numerical experiments for different number of iterations, the results of which are presented in Fig. 5.

We assumed here, that parameters values correspond to above mentioned ones, the constant of exchange interaction of the shell spin magnetic moments is  $J_S = -5$  K, the anisotropy constant is  $K_S = 20$  K. As seen from Fig. 5, with the growth of a number of iterations the desired dependences tend to the corresponding ones for the fixed spin magnetic moments of the shell. The differences in diagrams are caused, including, by the closely spaced quasi-equilibrium particle levels, differing by an ordering of the shell spin magnetic moments. For this problem solving it is necessary to carry out the large-sample averaging to take into account the main ensemble realizations.

#### **3.3** Dependences on the exchange interaction constant in the interface layer

With  $J_{If}$  growth by the magnitude the exchange bias field increases and the coercitivity decreases, since the shell spin magnetic moments are the "initiators" of the reversal process.

Hence, than the interaction through the interface layer is more intensive, that at smaller values of the external field the mass reorientation of the core spin magnetic moments takes place. It is interesting, that  $H_{EB}(J_{If})$ dependence is nonlinear: the considerable increase (by the magnitude) is observed in the ranges (2; 4) and (-4; -2) only. In the range of  $J_{If}$  values (-2; 2) the particle does not almost perform the exchange bias phenomenon whereas the coercitivity value within this interval is appreciably changed.



Fig. 5 – Dependences of the coercitivity  $H_C(1)$  and the exchange bias field  $H_{EB}(2)$  versus the particle radius. The number of iterations per spin:  $10^3$  (a);  $2 \cdot 10^3$  (b);  $5 \cdot 10^3$  (c)



**Fig. 6** – Dependences of the exchange bias field  $H_{EB}(1)$  and the coercitivity  $H_C(2)$  versus the exchange interaction constant  $J_{If}$  on the core-shell interface

# 4. CONCLUSIONS

Thus, in the present work the influence of the temperature, the core radius, and the exchange interaction constant in the interface layer on the coercitivity and the exchange bias field of the core-shell spin system is numerically studied. It has been established that the core ferromagnetic ordering destruction due to the temperature increase leads to the coercitivity disappearance and the exchange bias field decrease. It was shown that the coercitivity grows with the core radius. At the same time the exchange bias field strongly depends on the type of the interface layer formation and shows the non-monotonic dependence on the core radius. With the exchange interaction constant growth by the magnitude in the interface layer the exchange bias field increases and the coercitivity decreases.

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