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Magnetization Processes of Nanoparticles Embedded into Ferromagnetic Matrix

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The paper refers to computer simulations of interactions between magnetically hard particle embedded into ultra-hard matrix. We used simulated annealing and Monte Carlo simulations in a frame of the 3D Heisenberg model. The performed simulations reveal that the particles show additional exchange anisotropy dependent on "frozen" spin direction in the matrix and the angle between matrix and particle easy magnetization axes. The particle–matrix coupling are responsible for multi-phase magnetic hysteresis shape and exchange-bias like effect.

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1. Introduction

Magnetic materials are very important in nowadays technologies. Increasing requirements can be fulfilled by modern nanostructured magnetic composites containing different phases characterized by different magnetic properties. In the field of hard magnetics, interactions between the phases are especially important and can lead to an appearance of new and unique properties [1, 2]. Recently we have reported high coercivity in Fe–Nb–B–Tb group of bulk nanocrystalline alloys [3]. The alloys contain nanograins of magnetically hard ($Tb_2Fe_{14}B$) and relatively soft ($TbFe_2$,Fe) phases. In this case interesting is high value of coercive field (about 3.6 T) and asymmetric hysteresis loops. Moreover, the shape of the hysteresis suggests an occurrence of hard and ultra-hard magnetic phases, as shown in Fig. 1. Apart from the technical aspect of the obtained materials, the possible origin of the hysteresis shape is the main question. It was proposed an analysis for determination of apparent energy barrier and average magnetic moment of some magnetic objects that contribute to magnetization process. The conclusion was that (i) the observed magnetic hardening can be attributed to increasing role of inter-grain coupling and (ii) not all objects can be reversibly magnetized after the first saturation and these ultra-hard magnetic objects can be consider as additional source of exchange anisotropy. Therefore, a study concerning an influence of extremely hard magnetic surroundings on particle magnetization seems to be important [4–6].

The aim of this paper is to study a role of interactions between magnetically hard and ultra-hard particles. We used simulated annealing and Monte Carlo simulations in a frame of the 3D Heisenberg model and a setup described in the next section.

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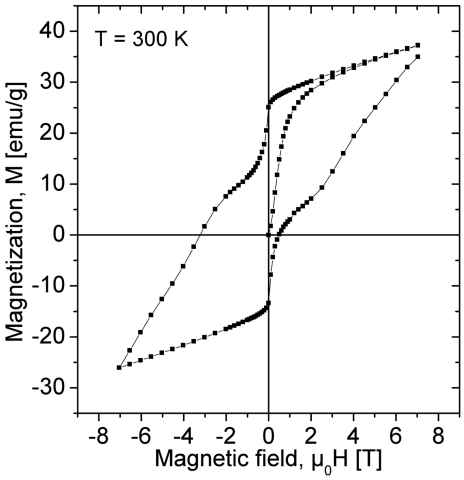

Fig. 1. Hysteresis loop for $(Fe_{80}Nb_6B_{14})_{0.88}Tb_{0.12}$ bulk alloy (for details see [3]).

2. Particle design and calculation procedure

The particle setup used in our simulations consists of a spherical particle embedded into cubic box. The particle diameter was 7 nm and it contains regularly placed spins with a distance of 0.2 nm in each directions. Around the particle there is a boundary space with a thickness of 0.5 nm with parameters that simulates particle–matrix coupling. Finally, there are $N = 1.25 \times 10^5$ spins in the system.

Energy of the system was calculated in the frame of the 3D Heisenberg model:

$$E = -\sum_{i,j} J_{ij} \boldsymbol{S}_i \boldsymbol{S}_j - \sum_i K_i \left(\boldsymbol{S}_i \cdot \boldsymbol{n}_i\right) - g\mu_{\mathrm{B}}\mu_0 \sum_i \boldsymbol{H}_i \cdot \boldsymbol{S}_i, \quad (1)$$

where J_{ij} is the exchange parameter, $\boldsymbol{S}_i$ is the spin vector on site i, K_i is the anisotropy constant (per site), $\boldsymbol{n}_i$ is the easy magnetization axis, g is the Landé factor, μ_{B} is the Bohr magneton, μ_0 is the vacuum permeability and $\boldsymbol{H}_i$ is the magnetic field on site i.

In order to determine magnetization of the system and spin configuration we used simulated annealing plus Monte Carlo, as briefly described below:

Step 1. Set (i) random orientation of the spin on each sites and (ii) initial annealing temperature.

Step 2. Choice a site and change, also at random, its spin orientation by a defined angle step.

Step 3. Calculate energy using the formula (1).

Step 4. If the energy of the new configuration is lower than before, accept the new configuration. If not, accept the new configuration with the probability $\exp\left(\frac{\Delta E}{\Delta T_{\mathrm{SA}}}\right)$, where ΔE is the energy change caused in step 2.

Step 5. Geometric decay of T_{SA} after $10N$ iterations. If T_{SA} is not a final temperature go to step 2.

Step 6. Keep the value of T_{SA} and calculate average magnetization of the system for $4000N$ iterations.

If in step 4 a new configuration is not accepted then the procedure starts to determine a cluster containing the chosen spin (using the Wang approach [7]), and next, perform the same one iteration changing spin orientation for the whole cluster. In our case there are three regions: particle ($J_{ij}^{\mathrm{P}} = 10^{-2}$ eV, $K_i^{\mathrm{P}} = 10^{-4}$ eV), boundary ($J_{ij}^{\mathrm{B}} = 10^{-5} - 5 \times 10^{-4}$ eV, $K_i^{\mathrm{B}} = 0$) and matrix ($J_{ij}^{\mathrm{M}} = 10^{-2}$ eV, $K_i^{\mathrm{M}} = 10^{-3}$ eV). For the whole system the spins equal 1. We analyzed three cases when easy magnetization axis of the particle is placed parallel, perpendicular and at 45° to the easy magnetization axis of the matrix which is also the direction of the external magnetic field. The J_{ij}^{B} parameter is directly responsible for the particle–matrix (P–M) coupling and its low values are an equivalent of the boundary region disorder and/or not perfect coupling (varying surface contact) that take place in real nanocomposite materials. The value of K_i^{M} where chosen to simulate ultra-hard magnetic phase i.e., the field up to ±5 T cannot change spin direction in the matrix.

3. Results and discussion

Figures 2–4 show results of the performed simulated hysteresis loops for different configurations of easy magnetization axes and different exchange parameters of the boundary region (named J in the figures) at "annealing temperature" $T_{\mathrm{A}} = k_{\mathrm{B}}T = 10^{-4}$ eV ($J_{ij}^{\mathrm{P}}/k_{\mathrm{B}}T = 100$). Magnetization of the particle was determined as average projection of spins to the z-axis (of the whole system and after subtraction of the matrix contribution). For the all analyzed cases one may observe significant shift of the hysteresis and appearing of their asymmetry. In a comparison with the classical non-interacting Stoner–Wohlfarth particle interesting is the results obtained for the perpendicular P–M configuration (see Fig. 4) where the stronger P–M coupling causes coercivity and exchange-bias effect (shift of hysteresis along H-axis). This means that the ultra-hard magnetic phase, that does not contribute directly to the magnetization process, can be a source of additional asymmetric anisotropy which in real materials may be an origin of exchange-bias effect.

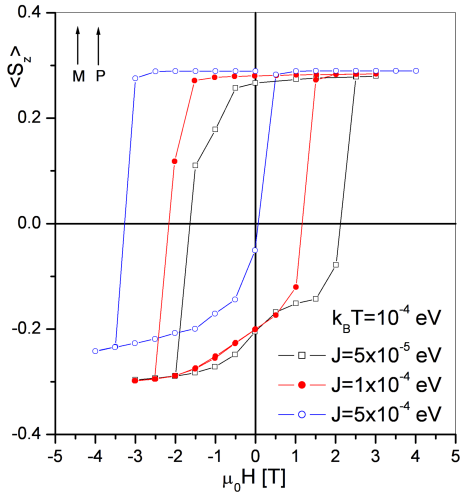

Fig. 2. Simulated hysteresis loops for parallel P–M anisotropy.

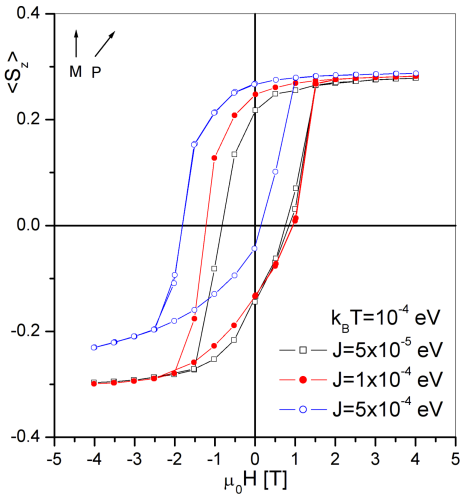

Fig. 3. Simulated hysteresis loops for 45° P–M anisotropy.

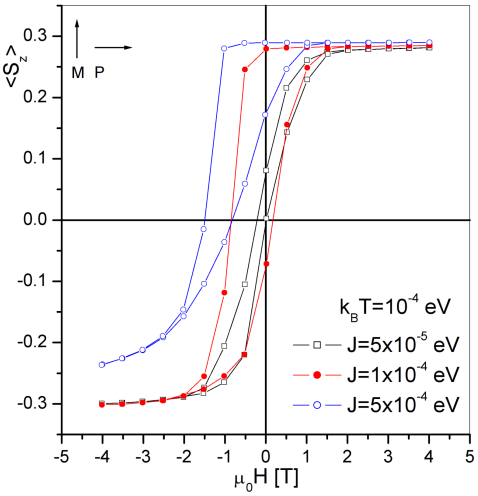

Fig. 4. Simulated hysteresis loops for perpendicular P–M anisotropy.

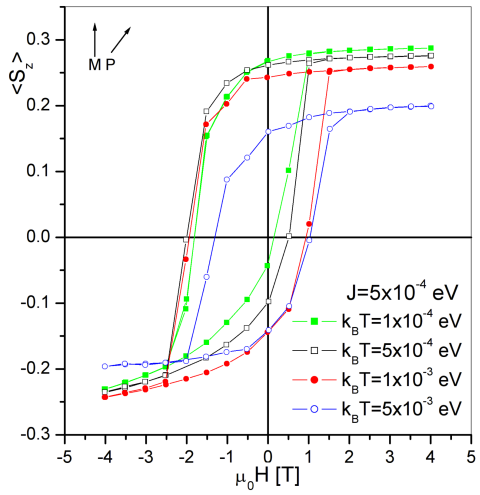

Fig. 5. Simulated hysteresis loops for 45° P–M anisotropy at different temperatures.

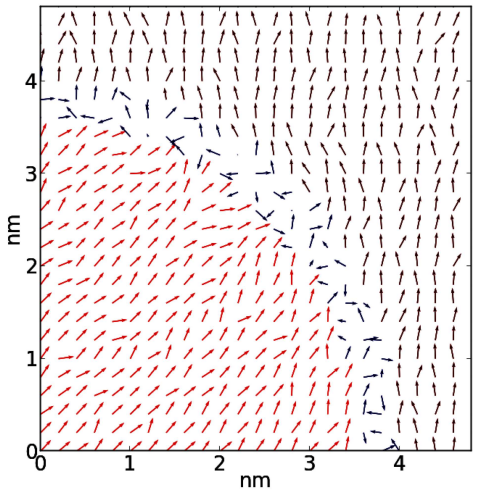

Fig. 6. Spin configuration (a quarter of central section) for $k_{\mathrm{B}}T = 5 \times 10^{-3}$ eV in the remanence point (the case as in Fig. 5).

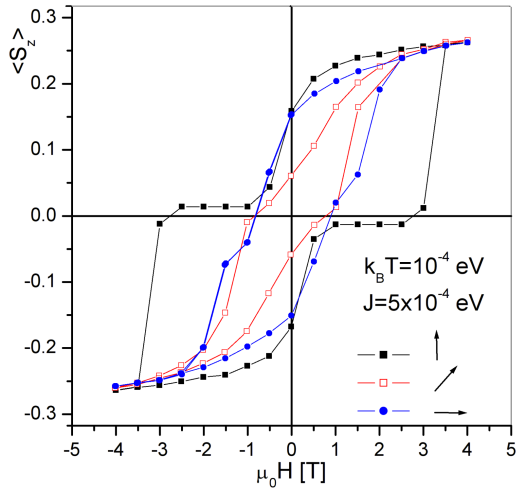

Fig. 7. Hysteresis loops for the whole P–M anisotropy configuration for the systems with parallel and anti-parallel matrix spins alignment.

Figure 5 depicts an influence of temperature on hysteresis loop for the considered particle–matrix system (the case of 45° P–M anisotropy). As shown, with the increase of temperature one may observed a decrease a saturation magnetization and the hysteresis becomes more symmetric. The explanation of this behavior is that the temperature causes a spin disorder in the boundary region and therefore, the additional exchange anisotropy is not related to the direction of easy axis of the matrix. Figure 6 shows the obtained spin configuration for $k_{\mathrm{B}}T = 5 \times 10^{-3}$ eV in the remanence point (the case as in Fig. 5) where the temperature effect on the boundary region is clearly visible.

In real magnetic nanocomposites, with random distribution of easy magnetization axes of the ultra-hard phase, one may find the cases when the spins are "frozen" parallel or anti-parallel to external magnetic field. Therefore, a shape of the hysteresis can be more complex than for non-interacting particle systems.

Figure 7 presents such a case for the three P–M configurations examined. In fact, for each studied case, the hysteresis reveals two magnetic phases originating from the same particle. The different anisotropy is attributed to different direction of "frozen" matrix spins. Comparing these results and the hysteresis in Fig. 1 one may conclude that some ultra-hard magnetic phase can be responsible for the observed multi-phase shape of hysteresis as well as exchange-bias like effect.

4. Conclusions

In relation to ferromagnetic system containing magnetically hard particles embedded into ultra-hard matrix the performed simulations reveal that: (i) the particles show additional exchange anisotropy dependent on "frozen" spin direction in the matrix as well as the angle between matrix and particle easy magnetization axes, (ii) the particle–matrix coupling are responsible for multi-phase magnetic hysteresis shape as well as exchange-bias like effect.

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