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Micromagnetic simulation of multiphase nanocrystalline material with different boundary conditions

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The micromagnetic formalism was used to study the magnetic behaviour of an assembly of single-domain ferromagnetic particles, with random easy axes of anisotropy, embedded in a weakly magnetic matrix. The results for various boundary conditions are compared.

Key words: *micromagnetic simulations; nanocrystalline material; hysteresis loop*

1. Introduction

Numerous magnetic materials used in modern technological applications are composed of fine magnetic particles either isolated or embedded in a non-magnetic or magnetic matrix. The analysis of multiphase systems is a difficult task, which has to include experimental studies as well as theoretical modelling. The complexity of the theoretical description of multiphase magnetic materials usually requires a numerical treatment. One of the possible approaches is the numerical micromagnetics that experiences the renaissance from the early 90th. The mathematical background of the micromagnetics [1] consists in the minimization of the magnetic free energy of a ferromagnetic material under certain conditions. Those "certain conditions" include parameters: (i) of the external environment influence such as applied field, temperature, stress; (ii) of the material (exchange integral, anisotropy constant, saturation magnetisation, etc.); (iii) of the system geometry that describe the sample (and in the case of non-uniform material its inner structure) as well as the boundary conditions for the micromagnetic problem.

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The calculations presented in this paper were performed for a peculiar nanostructure composed of randomly oriented crystalline grains, exhibiting high magnetic moment and strong uniaxial anisotropy, embedded in a weakly magnetic isotropic matrix.

2. Micromagnetic model

The system under consideration is a cube of the edge size D divided into $N\times N\times N$ cubic elements with the linear size d (see Fig. 1). Our calculations were performed for $N = 32$ or 64 and $d = 7$ nm. Various boundary conditions were considered: free, periodic in two dimensions and periodic in three dimensions. In the case of the free boundaries, the linear sample size is D and can be calculated by simple multiplying the size of the discretisation element by the number of elements, i.e., $D = dN$. However, for periodical boundary conditions the edge size D means the period size of the model and has nothing to deal with the sample physical size. In this case, the cube of linear size D is replicated infinite number of times in two or three dimensions. Thus, the periodical boundary conditions allow us to implement the infinite sample size in the model. The assumption of the "infinite size" gives two main advantages: there are no finite size effects and it is possible to compare the results achieved with experimental data of a corresponding bulk material.

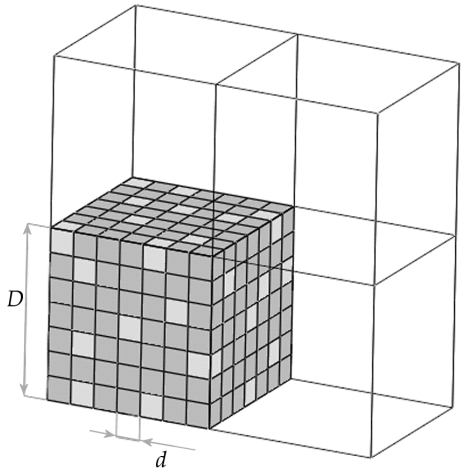

Fig. 1. Cubic discretisation procedure: D is the period size, d is the size of the discretisation element. Light cubes represent the grains embedded in matrix which is represented by dark cubes

Here and below, we consider the whole specimen as a finite or infinite regular mesh of closely packed interacting cubic elements [2]; discretisation cubic elements refers to mesh cells.

The mesh used for numerical calculations is a two-phase system that consists of crystalline particles with uniaxial anisotropy randomly embedded in a weakly magnetic isotropic matrix with the 10% packing density of grains. The size of each particle is the same and equals the cell size *d*. The directions of easy axes of particles are generated randomly with a uniform distribution of the direction cosines.

Since the size of the mesh cells is sufficiently small to meet the assumption of the micromagnetics (i.e., it is smaller than the exchange characteristic length), the magnetisation in each of them can be substituted for a classical vector. All calculations are carried out for low temperatures, where the thermal fluctuations can be neglected.

The considered magnetic free-energy functional includes the energy contributions from the field applied, uniaxial anisotropy, exchange and magnetostatic interactions

$$E_{\text{tot}} = E_{\text{app}} + E_{an} + E_{ex} + E_{\text{mag}}$$

The external field energy E_{app} and uniaxial anisotropy energy E_{an} terms are used in their classical forms [3]. The exchange energy is calculated by means of the Heisenberg-like term. The magnetostatic energy contribution E_{mag} is calculated using the explicit expression for demagnetising field presented by Nakatani et al. [4] and summed over the specimen by means of the Fast Fourier Transform (FFT) technique [5] with the aid of numerical routines called the Fastest Fourier Transform in the West [6].

Defining the magnetisation vector in the *i*-th mesh cell as

$$\mathbf{M}_i = M_S^{\sigma} \mathbf{m}_i$$

where M_S^{σ} denotes the saturation magnetisation of the σ sort of material, i.e., grain or matrix; $\mathbf{m}_i$ is the unitary vector parallel to magnetisation of the *i*-th cell, the total energy density of a sample in a uniform field applied is a sum of the energy densities of the mesh cells and can be written as

$$e = \sum_i e_i = -\sum_i \left[\left(\mathbf{H}_{\text{app}} \mathbf{M}_i\right) + \mathrm{K}_1^{\sigma} \left(\mathbf{n}_i \mathbf{m}_i\right)^2 + \frac{1}{d^2} \sum_{\delta i} \mathrm{A}_{i,\delta i} \left(\mathbf{m}_i \mathbf{m}_{\delta i}\right) - \frac{1}{2} \left(\mathbf{H}_i^D \mathbf{M}_i\right) \right]$$

where $\mathbf{H}_{\text{app}}$ is the applied field, K_1^{σ} – anisotropy constant and *n* is the easy-axis direction vector; $A_{i,\delta i}$ – exchange constant, where δi means the number of neighbours to the *i*-th node; $\mathbf{H}^D$ – demagnetising field.

The minimization procedure is provided by the Jacobi iterative scheme based on the Landau–Lifshitz equation of motion for magnetic moments without a precession term [7], i.e.

$$\frac{d\mathbf{m}_i}{dt} = -\mathbf{m}_i \times (\mathbf{m}_i \times \mathbf{h}_i^{\text{eff}})$$

where the time scale includes the factor preceding the vector product, and $\mathbf{h}^{\text{eff}}$ is the effective field defined as

$$\mathbf{h}_i^{\text{eff}} = -\frac{\partial e_i}{\partial \mathbf{M}_i}$$

The condition for the equilibrium state of magnetisation is the requirement that for every node the magnetisation vector should be parallel to the appropriate effective field that gives a minimum of the magnetic free energy. Thus, to achieve the equilibrium one should recalculate the effective field and use the Landau–Lifshitz equation to gain the next transition state for each iteration step.

3. Results

The material parameters used for the appropriate calculations are presented in the table. These parameters were chosen so as to approximately correspond to the recently produced and experimentally studied $Co_{66}Nb_9Cu_1Si_{12}B_{12}$ nanocrystalline material, obtained by the isothermal annealing of the amorphous alloy [8]. We have already used this material as a basis for the comparison of numerical results with the experimental data that revealed a good qualitative agreement [9].

Table. Material parameters used for the micromagnetic calculations

	A, erg/cm	K_1, erg/cm^3	M_S, emu/cm^3
Grains	10^{-6}	2.7×10^6	1360
Matrix	0.2×10^{-6}	0	160
Matrix–grain interface	0.2×10^{-6}	–	–

The hysteresis loops obtained for the nanostructure studied in the case of the free boundary conditions as well as periodic in 2 and 3 dimensions are presented in Fig. 2 and Fig. 3 for the mesh sizes $N = 32$ and 64, respectively.

It has been already shown that in such a nanostructure, due to the exchange coupling between the highly anisotropic crystallites and the surrounded isotropic matrix, the material is combined into randomly oriented weakly related clusters [9]. The results of the simulations of magnetisation processes indicate that during the magnetisation reversal process the clusters reverse sequentially in a reversal field, which can be considered as an external field modulated by a magnetostatic field from the neighbouring clusters. For clusters which are preferentially adjacent parallel to the applied field the reversal field is enhanced, whereas for transversally adjacent clusters it is reduced. This results in a step-like shape of the hysteresis loops presented in Figs. 2 and 3. Depending on the strength of the exchange coupling via the grain–matrix interface and the anisotropy constant of the grains, one can obtain a cluster structure that is stable during the whole reversal process (as in this work) or unstable clusters for which the magnetisation of the matrix tears off from the grains in high enough reversal field [9].

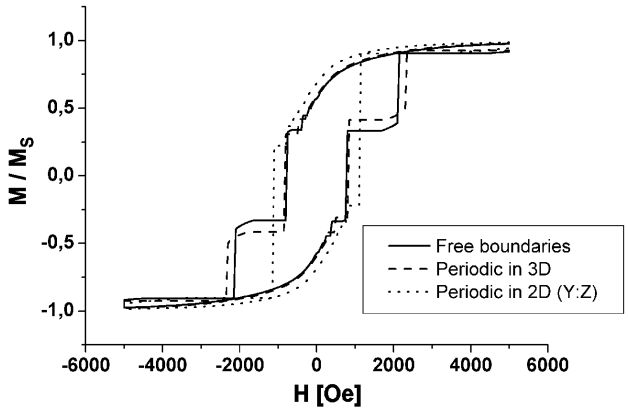

Fig. 2. Hysteresis loops calculated for different boundary conditions.
Sample mesh size is 32×32×32 nodes.
The direction of the external field is parallel to the *z*-axis

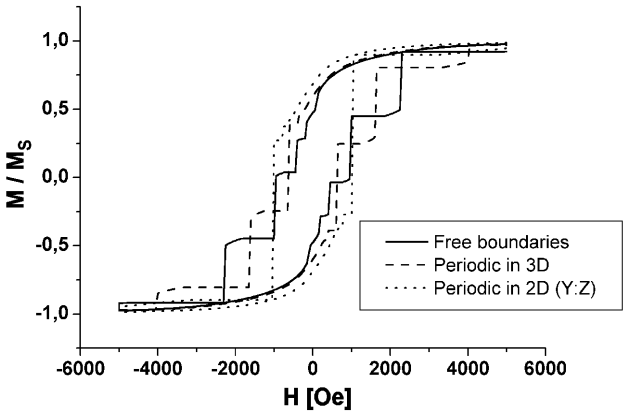

Fig. 3. Hysteresis loops calculated for different boundary conditions.
Sample mesh size is 64×64×64 nodes.
The direction of the external field is parallel to the *z*-axis

For a certain mesh size, the different shapes of the calculated loops are the consequences of the various levels of the finite-size effects. In the case where there is at least one non-periodic dimension, on the free faces of a nano-sample the surface magnetic poles can appear. These additional magnetic poles increase the demagnetising field, which, in turn, modifies the magnetisation reversal. The periodicity removes these finite-size effects, so the resulting hysteresis loop can be compared to the experimental one measured for a macro-sample. The 2*D* periodic boundary conditions can be applied to modelling thin magnetic films. However, this approximation is not sufficient for bulk materials for which the rotational processes, which occur at higher fields, are lost. The increase of the mesh size leads to the refinement of the loop shape due to the improved averaging of the magnetisation over larger number of grains. In

this case, one can obtain a better approximation of the experimental results but, on the other hand, the increase of the mesh size substantially increases the calculation time.

4. Conclusions

It has been shown that the magnetic properties of the system consisting of ferromagnetic particles with high uniaxial anisotropy strongly depend on the magnetic state of the matrix in which they are dispersed. The presence of a small matrix magnetic moment and weak, both in-matrix and matrix-crystallite, exchange couplings lead to cluster-like inner magnetisation patterns. The magnetisation reversal in such nanostructure proceeds by sequential rotation of magnetic moments within the clusters. The shape of the calculated hysteresis loop, which represents this magnetisation process, strongly depends on the boundary conditions, which should carefully be chosen for the simulation of the real experiment.

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