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A New Approach to Determination of Equilibrium Magnetization in Magnetic Nanostructures

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A new approach to determination of the equilibrium magnetization in discrete model of a ferromagnetic is presented. Solving this problem is reduced to a system of linear inhomogeneous equations with Lagrange multipliers. The possibility of finding the numerical solutions of such systems is shown by applying of a modified power method. The efficiency of this approach is proved by examples of modelling magnetic microstructure and magnetization reversal process in a nanostructured thin magnetic film.

Keywords: micromagnetics, numerical analysis, magnetic hysteresis, magnetic domains, nanostructures.

Introduction

Determination of the equilibrium configuration of magnetic moments is the base of micromagnetic modeling, and plays a key role in studying magnetic microstructures [1, 2], processes of magnetization reversal [3, 4], in calculation of magnetic normal modes [5] and absorption spectra [6] in nanostructures. There exist different methods to find the equilibrium configuration [7].

The commonly used approach based on performing a Runge-Kutta integration of the Landau-Lifshitz equation with a damping term is very popular due to its physical transparency, guaranteed convergence and large experience accumulated in numerical analysis for solving systems of ordinary differential equations. But this method has numerous disadvantages. The major ones are interrelated problems — the magnetization length preserving and the long calculation time [8].

The Monte-Carlo approach is the most efficient method for the global energy minimization. However this approach becomes very slow for more than a few dipoles.

The third approach is the total-energy minimization method. Its algorithm is based on some standard numerical methods for the minimization of multivariable functions. The constraint of the dipole's length makes this problem nonlinear and very difficult for estimating convergence.

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The most successful method involves organization of an iteration procedure based on the fact that in the equilibrium state the magnetization should be aligned parallel to the corresponding effective field. In this method one can occasionally get trapped by repetitively jumping between two unstable configurations [9]. But for most situations it proved to be the fastest and the most reliable method.

Here we present a new efficient approach to find the equilibrium configuration which is, inherently, a development of ideas of the last one.

1. Discrete Dipole Approximation Model

Our approach is based on the model involving N discrete dipoles $\vec{\mu}_i$ (i=1,2,...,N), often called the discrete dipole approximation. In this model a sample is divided into equal cells, the magnetization is assumed to be uniform in each cell, and that each dipole precesses about its equilibrium direction under the influence of the external and magnetic anisotropy fields, the dipolar and exchange forces. Taking into account the following notations: cell's volume V, the saturation magnetization M_s and dipole's direction $\mathbf{m}_i$ (i.e., $\vec{\mu}_i = M_s V \mathbf{m}_i$), the free energy density can be written as a sum of Zeeman, exchange, magnetic anisotropy and dipolar energies

$$E(\mathbf{m}_1, \mathbf{m}_2, \ldots, \mathbf{m}_N) = -M_s \mathbf{H} \sum_{i=1}^{N} \mathbf{m}_i + J \sum_{i=1}^{N} \sum_{j=1}^{Ni} (1 - \mathbf{m}_i \mathbf{m}_j) +$$

$$+ \frac{M_s^2 V}{2} \sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} \left[\frac{\mathbf{m}_i \mathbf{m}_j}{r_{ij}^3} - \frac{3(\mathbf{m}_i \mathbf{r}_{ij})(\mathbf{m}_j \mathbf{r}_{ij})}{r_{ij}^5} \right] - \sum_{i=1}^{N} K_i (\mathbf{m}_i \mathbf{n}_i)^2, \qquad (1)$$

where $\mathbf{H}$ is external field, J is the exchange constant, and the second sum extends over the nearest neighbors Ni of cell i, $\mathbf{r}_{ij}$ is the radius-vector between the ith and the jth cells, K_i is the anisotropy constant, and $\mathbf{n}_i$ is the unit vector of the easy magnetic axes direction of the cell i. The inclusion of other energy terms (like surface anisotropy or magnetoelastic energy) is possible, but we are not going to consider them here.

The equilibrium condition for this system is a stationarity of the energy E, i.e., $\delta E(\mathbf{m}_1, \mathbf{m}_2, \ldots, \mathbf{m}_N) = 0$ under the constraint of the dipole magnitude ($m_{ix}^2 + m_{iy}^2 + m_{iz}^2 = 1$, $i = 1, \ldots, N$). The solution of this variational problem by Lagrange multiplier method is reduced to the system

$$\mathbf{H}_k^{eff}(\mathbf{m}_1, \mathbf{m}_2, \ldots, \mathbf{m}_N) - \nu_k \mathbf{m}_k = 0, \qquad (2)$$

where $\mathbf{H}_k^{eff} = -\frac{1}{M_s} \frac{\delta E}{\delta \mathbf{m}_k}$ is an effective local magnetic field, ν_i are the Lagrange multipliers. From the physical point of view, these equations show that in the ground state each dipole is parallel to the corresponding effective field. And Lagrange multipliers ensure the dipole length constant.

The influenced on dipole k effective local magnetic field $\mathbf{H}_k^{eff}$ is a linear function all magnetic dipoles $\mathbf{m}_i$ ($i = 1, 2, \ldots, N$):

$$\mathbf{H}_k^{eff}(\mathbf{m}_1, \mathbf{m}_2, \ldots, \mathbf{m}_N) = \mathbf{H} + \frac{2J}{M_s} \sum_{j=1}^{Ni} \mathbf{m}_j +$$

$$+ M_s V \sum_{j=1, j\neq k}^{N} \left[\frac{3\mathbf{r}_{kj}(\mathbf{m}_j \mathbf{r}_{kj})}{r_{kj}^5} - \frac{\mathbf{m}_j}{r_{kj}^3} \right] + \frac{2K_k}{M_s} (\mathbf{m}_k \mathbf{n}_k) \mathbf{n}_k \,. \qquad (3)$$

Therefore the system (2) can be rewritten in the matrix form:

$$A\mathbf{x} - D\mathbf{x} = \mathbf{b}, \tag{4}$$

where $\mathbf{x} = (m_{1x}, m_{1y}, m_{1z}, m_{2x}, m_{2y}, \ldots, m_{Nz})^T$, T denotes transposition,

$$D = \mathrm{diag}(\nu_1, \nu_1, \nu_1, \nu_2, \nu_2, \nu_2, \nu_3, \ldots, \nu_N)$$

is the diagonal matrix, the column vector $\mathbf{b}$ and symmetrical matrix A are characterized by system properties (3).

Solving the equilibrium configuration problem in the form (4) has a number of advantages. It enables one to use comprehensive facilities of numerical algorithms of the linear algebra, to take advantages of sparse matrices and parallel computing.

In this work we used the simplest power-like iterative scheme

$$\mathbf{y}_{i+1} = A\mathbf{x}_i - \mathbf{b}, \tag{5}$$

$$\mathbf{x}_{i+1} = D_{i+1}^{-1}\mathbf{y}_{i+1}\,. \tag{6}$$

At the first step we find effective local magnetic fields, and at the second we normalize the vector $\mathbf{x}$ in the special form: $|\mathbf{m}_i| = 1$, $i = 1, 2, \ldots, N$.

It was significant to note that the convergence condition of the process is the positive definiteness of matrix A. This can always be done by solving the equivalent problem $A'\mathbf{x} - D'\mathbf{x} = \mathbf{b}$, where the positive-definite matrix $A' = A + \xi E$, $D' = D + \xi E$, E is unity matrix, and $\xi > 0$.

2. Numerical Simulation

For demonstration of an efficiency of this approach we have modeled magnetic microstructures and magnetization reversal on the model of thin magnetic film considered in [2]. According to this paper, the film is a system of closely packed 2.5 nm ferromagnetic grains with a random distribution of uniaxial anisotropy axes. Exchange interaction between grains is described by an effective exchange constant J_{eff}. The behavior of the system is governed by the single parameter $\gamma = J_{eff}/K$ (where K is magnetic anisotropy constant) i.e., the ratio between the exchange and anisotropy energies.

The simulation based on eq.(4) was performed on a desktop PC for one layer of 50×50 nanoparticles in size in the absence of the external magnetic field. In order to exclude the influence of the boundary conditions, the presented patterns (Fig.1) correspond to the configurations of the internal region 20×20 in size. We used the following parameters of the model: a random distribution of uniaxial anisotropy axes in the plane film, the magnetic anisotropy constant $K = 8 \cdot 10^5 \mathrm{erg/cm}^3$ and the saturation magnetization $M_s = 495\mathrm{G}$. Fig. 1*a*,*b*,*c* were obtained without dipole-dipole interaction for γ=0,1,2 respectively (CPU time $\sim$ 2 sec) and figure 1*d* — with dipole-dipole interaction for γ=1.25 (CPU time $\sim$ 1.5 min). Comparing the results on Fig. 1 with the similar ones from [2], it can be seen a good agreement.

Fig. 2 presents the results of the analogous calculation for equilibrium configurations of magnetic dipoles in the film with a space random distribution of uniaxial anisotropy. It should be taken into account that the dipole-dipole interaction leads to the preferred orientation of magnetic dipoles in the film plane. Also, we perform the calculation of magnetic-hysteresis loops for the thin films with previous model parameters and γ=0.75, 1.25. The results are shown on Fig. 3.

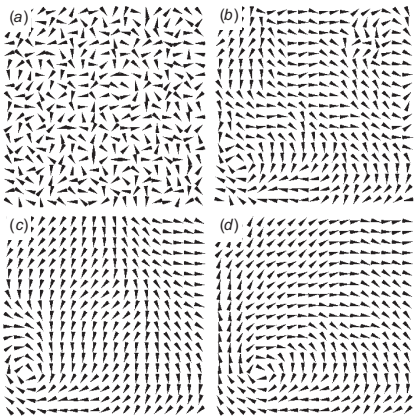

Fig.1. The equilibrium configuration of magnetic dipoles in the film with a plane random distribution of uniaxial anisotropy. a,b,c — without dipole-dipole interaction for γ=0,1,2 respectively, d — with dipole-dipole interaction for γ=1.25

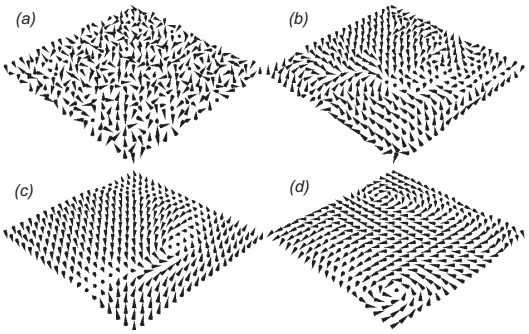

Fig.2. The equilibrium configuration of magnetic dipoles in the film with a space random distribution of uniaxial anisotropy. a,b,c — without dipole-dipole interaction for γ=0,1,2 respectively, d — with dipole-dipole interaction for γ=1

3. Conclusion

We have offered a new approach for determination of the equilibrium magnetization in discrete model of a ferromagnetic. The problem definition in the matrix form (4) gives us new opportunities. In particular, it enables us to use the comprehensive facilities of numerical algorithms of the linear algebra.

We have demonstrated the efficiency of this approach on a model of nanostructured thin magnetic film with a random distribution of uniaxial magnetic anisotropy axes by calculating magnetic microstructures and magnetization reversal of the film. The calculation results are in good agreement with the results obtained by other authors.

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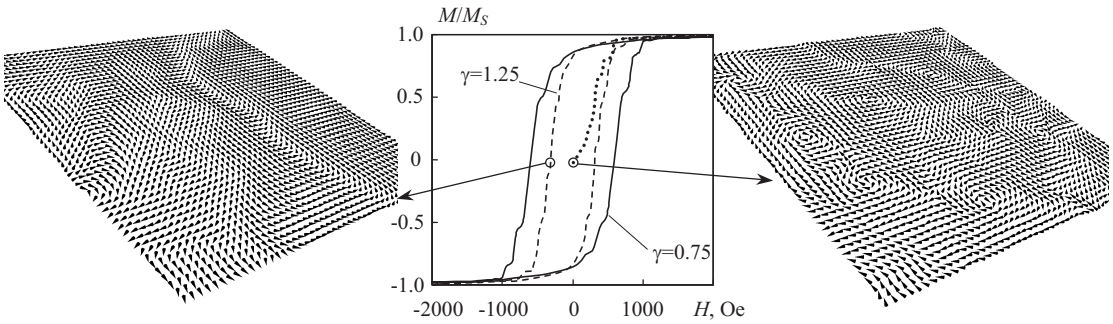

Fig.3. Calculated magnetic-hysteresis loops for the thin films with γ=0.75, 1.25 and magnetic microstructures for two different points of the loop

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Новый подход к определению равновесного состояния намагниченности в магнитных наноструктурах

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Представлен новый подход к определению равновесного состояния намагниченности в дискретной модели ферромагнетика. Для решения этой проблемы мы сводим ее к системе линейных неоднородных уравнений с множителями Лагранжа. Возможностъ нахождения численных решений таких систем показана применением модифицированного степенного метода. Эффективностъ данного подхода подтверждается примерами моделирования магнитной микроструктуры и процессов перемагничивания в наноструктурированной тонкой магнитной пленке.

Ключевые слова: микромагнетизм, численный анализ, магнитный гистерезис, магнитные домены, наноструктуры.