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Computer simulation application for improving correctness of data obtained by magnetic force microscope

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ABSTRACT

A method of a computer analysis of MFM images was developed. The computer analysis of MFM images of separate ferromagnetic single-domain nanoparticles placed on a nonmagnetic substrate was carried out. The shape of an MFM tip and the trajectory of its movement were taken into account. The aureoles were found in the magnetic contrast of MFM images simulated for the lifting mode. The conditions and the reasons of the appearance of these aureoles were discussed.

Keywords: Computer simulation, magnetic force microscopy, lifting mode, nanoparticle

1. INTRODUCTION

Recently a special attention is paid to investigating the properties of ferromagnetic nanoparticles because there is a possibility to create recording and storing devices of new generation on their basis[1,2]. The magnetic force microscopy (MFM) has a great potential for investigating the magnetic properties of surface ultra-small magnetic structures with rather high resolution and sensitivity. An MFM image contains information about the distribution of magnetization in a sample.

However, the interaction between a magnetic tip and a magnetic field created by surface structures is rather complex. Therefore it is often difficult to explain experimental MFM data. Special complexities occur in cases when samples with a rather developed relief are studied. Samples with separate ferromagnetic nanoparticles formed on a nonmagnetic substrate can be considered as such an object of investigation.

In this work a method of computer analysis developed earlier is applied to study the influence of the features of the tip movement on the formation of MFM images of a ferromagnetic single-domain nanoparticle.

2. PROCEDURE OF THE SIMULATION OF MFM IMAGES

The magnetic force microscope functions on the basis of registering the interaction between the magnetic tip and the magnetic field created by surface ferromagnetic structures[3-6]. To increase the sensitivity the oscillating mode of the microscope is widely used. In this mode a cantilever is put into forced oscillations on its eigenfrequency. In this case the changes of the following parameters of oscillations are registered: an amplitude, a frequency or an initial phase.

In the case of small oscillations and weak interactions the following expression holds[7]:

$$\Delta j = -\frac{Q}{k}\frac{\partial F_z}{\partial z} \qquad (1)$$

where *?f* is the phase shift due to the influence of magnetic forces, *Q* is the quality factor of the cantilever, *k* is the constant of elasticity of the cantilever, and $?F_z/?z$ is the *Z* component of the magnetic force gradient acting on the MFM tip in the given point of the spatial location of the tip.

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According to Eq. (1), the phase shift is proportional to the magnetic force gradient, so it is enough to calculate the gradient values in every point of the tip location over the investigated surface where the tip is situated during scanning. A two-dimensional matrix of the calculated values of the gradient represents the simulated MFM image.

To simplify the computation of the gradient it is considered that an external magnetic field created by the tip does not influence the sample magnetization, and vice versa. The magnetization structure of the tip and the sample depends on the geometry, magnetic properties and magnetic prehistory of each object and can be calculated in terms of the micromagnetic theory[8,9].

To calculate the gradient, magnetic capacities of the tip and the sample are divided into physically small areas. Every area is approximated by a point magnetic dipole the direction of which depends on the local magnetization structure and its magnitude is chosen for reasons of magnetic saturation and uniform magnetization of each local area. In this case, the gradient in the point **r** is calculated according to the following expression:

$$\frac{\partial F_z(\mathbf{r})}{\partial z} = \sum_{\substack{i-tip \\ j-sample}} \left(\left(\mathbf{m}_t^i \nabla\right) \frac{\partial H_z^{ij}\left(\mathbf{r} + \mathbf{r}_t^i - \mathbf{r}_s^j\right)}{\partial z} \right) \tag{2}$$

where $\mathbf{m}_t^i$ is the *i*-th magnetic dipole of the tip, H_z^{ij} is the *Z* component of the magnetic field, created by the *j*-th magnetic dipole of the sample in the point of spatial location of the *i*-th dipole of the tip, $\mathbf{r}_t^i$ and $\mathbf{r}_s^j$ are the coordinates of the corresponding magnetic dipoles in the systems of coordinates concerned with the corresponding objects. It is convenient to carry out the calculations when the system of coordinates of **r** is connected with the sample.

The software was recently developed by us to simulate MFM images of different ferromagnetic structures with known geometrical parameters and magnetization structure. This software is based on the described algorithm and allows one to take into account the real shape of the tip and the sample structures, and also to use the magnetization structures of both objects calculated with the micromagnetic theory beforehand. This software was successfully tested in theoretical and experimental investigations of different ferromagnetic micro- and nanostructures[10-12].

The process of scanning is modeled by the virtual displacement of the tip relative to the sample according to the trajectory of its movement. The virtual displacement of the tip consists in the changing of all relative coordinates of all local dipoles of the tip in the coordinate system connected with the sample. The changes of *X* and *Y* components of the spatial coordinates are accomplished step-by-step to form the image. The step-by-step change of *Z* coordinates of the dipoles depends on the features of the trajectory of the tip movement during scanning. It is especially important to take into account these features for the analysis of MFM images of relief objects.

In practice, two modes of the tip motion are often used: the mode of the constant distance and the lifting mode. In the first case the tip lifts up on the prescribed distance and this *Z* position remains constant. The trajectory of the tip movement can be described by a plane in this case. In the lifting mode the tip scans the same line of the image twice. At first the tip touches the surface and the line of the surface relief is registered. This profile is memorized in the control device. Then the tip lifts up and moves according to this profile not touching the surface and the main interaction becomes to be magnetic. In this case the trajectory of the tip movement differs from the plane and depends both on the real topography of the surface an on the shape of the MFM tip. Besides, if the surface has a developed relief, it is necessary to take into account the convolution effect of the real topography of the surface and the tip shape[13-15].

Both modes of the tip moving can be taken into account in the developed software. The distortions of a topography image caused by the convolution effect can also be taken into consideration. This fact allows us to provide a computer comparative analysis of an influence of trajectory of the tip motion during scanning on the formation of MFM images of the surface with separate ferromagnetic nanoobjects having the developed relief.

3. COMPUTER EXPERIMENT AND DISCUSSION OF RESULTS

The computer experiment was carried out to study of the influence of the features of the tip motion during scanning on the formation of MFM images of relief nanoobjects. A separate ferromagnetic nanoparticle in a uniformly magnetized state formed on a nonmagnetic substrate was taken as an object of research. The shape of the particle was taken to be cylindrical (Fig. 1*a,c*) 100 nm in the height and 50 nm in the radius. The specific magnetization was taken to be equal to 490 Oe/cm^3. The magnetization of the particle was directed along the surface or perpendicularly to the axis of the symmetry of the tip (Fig. 1*a*).

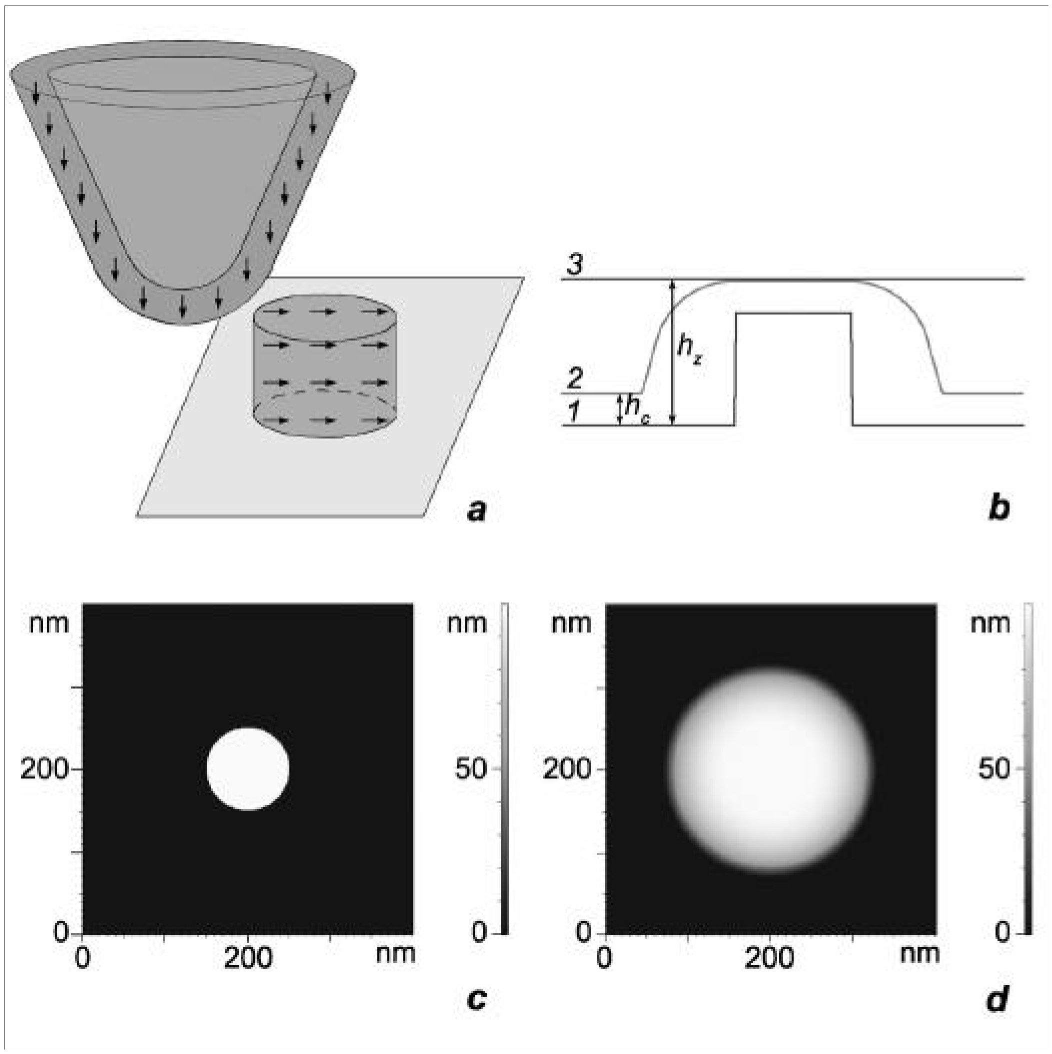

Figure 1. Models of a ferromagnetic nanoparticle and an MFM tip. *a* – the geometrical shapes and the structures of magnetization of the tip and the particle; *b* – the profiles: *1* – of the topography of the sample surface, *2* – of the trajectory of the tip movement in the lifting mode, *3* – of the trajectory of the tip movement in the constant distance mode; *c* – the top view of the topography of the sample surface with the nanoparticle; *d* – the simulated image of the topography presented in c distorted by the convolution effect.

The tip was approximated by a nonmagnetic truncated cone with the convergence angle of 30°. The apex of the cone was made round with the rounding radius of 20 nm (Fig. 1*a*). This nonmagnetic part of the tip was covered evenly by thin ferromagnetic coating with the thickness of 50 nm and the specific magnetization of 1700 Oe/cm^3. To simplify the following calculations it was supposed that the tip was also uniformly magnetized along its axis of symmetry. This model of the tip rather well describes tips widely used in real MFM experiments. Since the magnetic interaction strongly decreases as the distance between interacting objects increases, one can reliably consider that only a comparatively small part of the apex of the tip takes part in the formation of an MFM image. According to the results obtained in Ref. 11, it is enough to take the height of the nonmagnetic part of the tip to be equal to 200 nm for correct modeling. The simulation of MFM images was carried out in terms of the described techniques. For the calculations the magnetic part of the tip was divided into 4842 local magnetic dipoles and the nanoparticle consisted of 800 dipoles.

Two runs of MFM images for two modes of the tip motion were obtained. The MFM images were simulated for different distances between the tip and the sample surface in each run. The first lot of the images was obtained for the constant-distance mode with changing of this distance h_z. These images for several values of h_z are presented in Fig. 2*a*,*b*,*c*. Every MFM image contains the information about the existence of two magnetic poles of the nanoparticle and about their location. In workmanlike manner the presented images weakly differ from the results of simulation carried out with such objects under the assumption that the tip was approximated by a point magnetic dipole[10]. The analysis of the images obtained for the different values of the distance h_z confirmed the obvious conclusion that the resolution and the sensitivity of MFM decrease, as the distance between the tip and the sample surface increases.

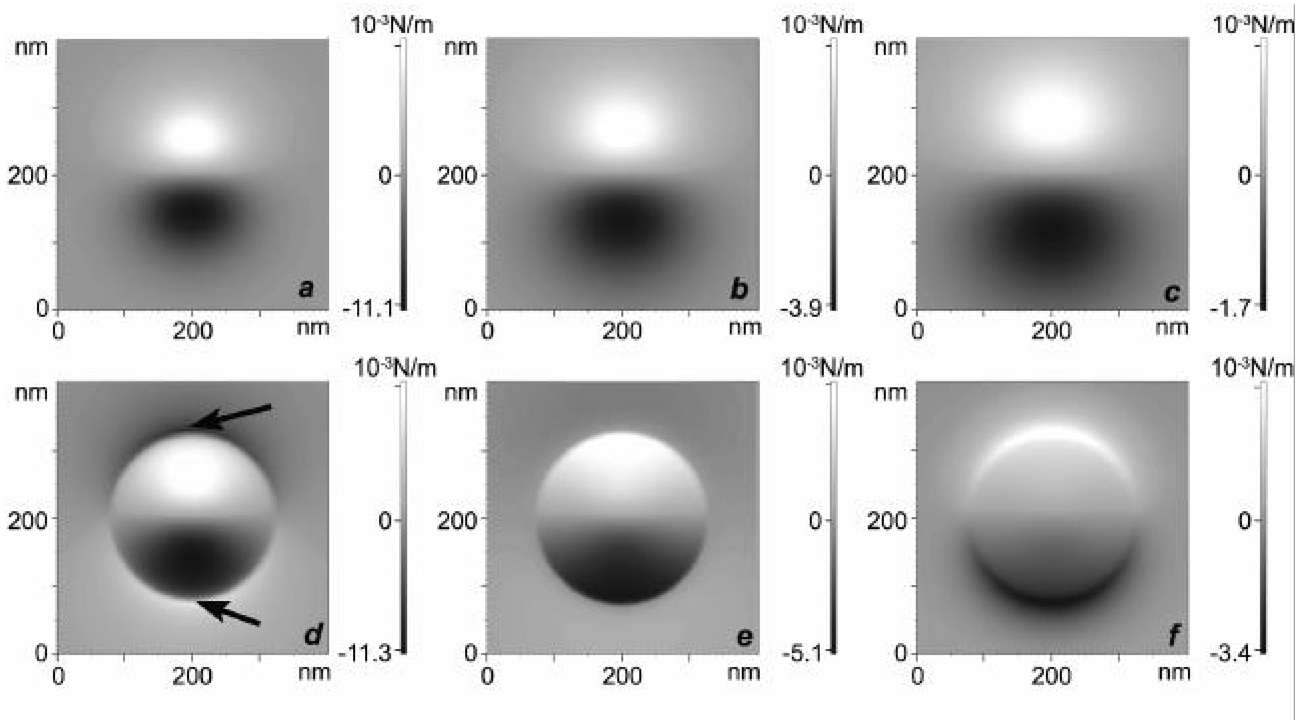

Figure 2. MFM images simulated for the constant-distance (a, b, c) and lifting modes (d, e, f) for different values of distances h_z and h_c. These values were the following: a – h_z=140 nm; b – h_z=180 nm; c – h_z=220 nm; d – h_c=40 nm; e – h_c=80 nm; f – h_c=120 nm. The gray scale represents different magnitudes of the force gradient of the magnetic interactions acting between the tip and the magnetic field created by the nanoparticle. This gradient was taken with the opposite sign according to Eq. (1). The arrows highlight the aureoles.

The second lot of the MFM images was simulated for the lifting mode of the tip motion for different lifting distances h_c. Several obtained MFM images are presented in Fig. 2*d*,*e*,*f*. These images differ in a workmanlike manner from the images obtained for the constant-distance mode. It is obvious that the more complex movement of the tip influences the formation of an MFM image, thereby this motion complicates the image. It is necessary to note that the magnetic contrast from the particle which was observed on the images exceeds a topography image of the nanoparticle. If the lifting distance was essentially smaller than the nanoparticle height, the magnetic contrast which described the magnetic poles at the edges of the object acquired a more complicated character, namely, the areas of the anticontrast arose. This area of anticontrast looked like aureoles (Fig. 2*d*). If the lifting distance increases, the aureoles disappear.

We suppose that the origin of these aureoles is as follows. If the lifting distance is less than the height of the particle, the apex of the tip is situated below the level of this height a the tip approaches the particle. As a result some part of the local dipoles of the tip and the local dipoles of the sample begin to interact with the sign which is opposite to that of the most part of the interactions which are contained in sum (2). These "negatively" interacting dipoles are situated closer than the "positively" interacting ones. The number of "negatively" interacting dipoles decreases as the lifting distance increases. That is why the aureoles can be observed only for the limited range of the lifting distances. The higher limit of this range depends on the shape of the tip and of the nanoobject and also on the structure of their magnetization.

The aureole appearance was observed in real MFM experiments carried out with the samples containing separate nickel nanoparticles formed on the surface of silicon dioxide[10]. Fig. 3 presents an MFM image of nickel nanoparticles obtained in the lifting mode in the presence of a small additional magnetic field directed along the sample surface. It can seen that the magnetic contrasts of some single-domain particles contain aureoles. It is also clear that the magnetic contrasts of the smaller nanoparticles have a good agreement with the simulated data obtained for the lifting mode in case of relatively high lifting distance (Fig. 2*f*) but not for the constant distance mode (Fig. 2*c*).

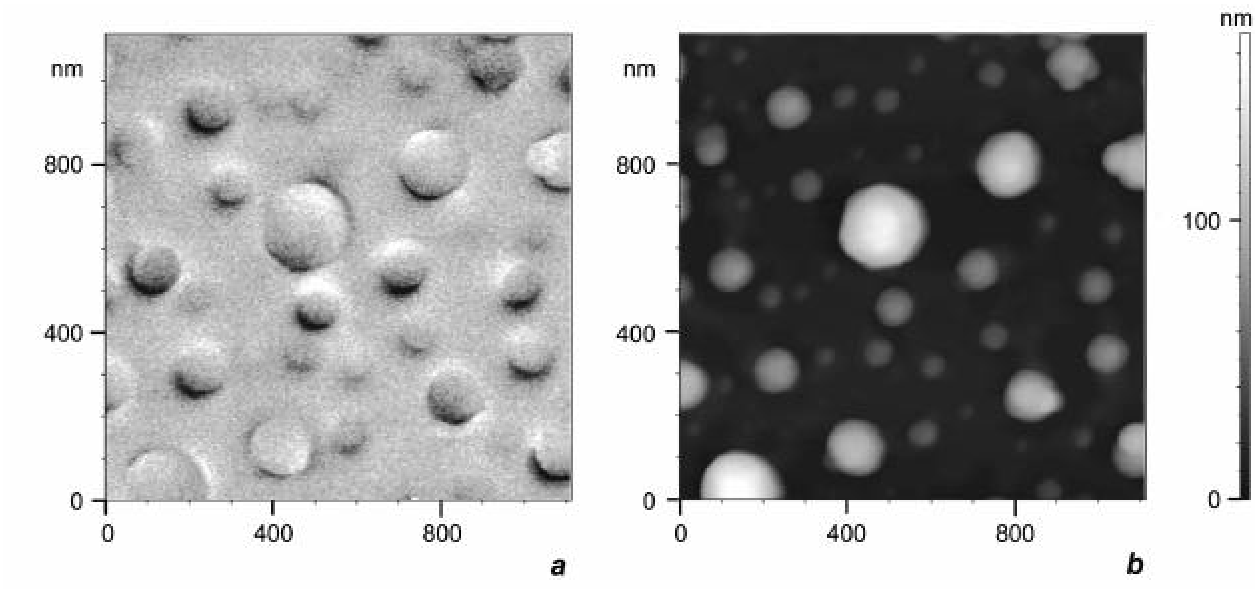

Figure 3. MFM image (*a*) and the topography (*b*) of an area of a sample with separate nickel nanoparticles formed on the silicon dioxide surface.

4. CONCLUSION

MFM images of ferromagnetic nanoparticles taking into account shapes of the MFM tip and nanoobject, the trajectory of the tip movement in the lifting mode and the convolution effect were simulated. The aureoles on the magnetic contrast in images obtained in the lifting mode, when the lifting distance was rather small, was clearly discernible. The appearance of the aureoles was explained by the existence of the "negative" interaction between the tip and the nanoparticle when the tip approaches the nanoparticle. The results of the computer analysis coincide in a workmanlike manner with the experimental data obtained earlier.

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