MICROMAGNETIC MODELING OF HYSTERESIS CHARACTERISTICS OF SUEVITES OF THE ZHAMANSHIN IMPACT CRATER

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Abstract. On the basis of coordinated theoretical modelling using two independent models that take into account possible chemical inhomogeneity of particles and magnetostatic interaction between them, we calculated the hysteresis characteristics of suevites of the impact crater Zhamanshin corresponding to the experimental data and estimated the concentrations of ferrimagnetic particles in the samples.

Keywords: *suevites, micromagnetic modeling, two-phase particles, magnetostatic interaction, superparamagnetism, frequency-dependent susceptibility, nanoparticle, magnetometry, magnetite, maghemite, hematite*

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INTRODUCTION

Micromagnetism is a macroscopic theory describing magnetization processes on length scales in the range of a few nanometers and more, when it is possible to disregard the discreteness of spins and consider magnetization as a continuous function of coordinates. By doing so, the number of calculations can be reduced by replacing the consideration of a huge number of spins with a substantially smaller number of finite elements. The theory of micromagnetism began with a paper by L. D. Landau and E. M. Lifshitz [1]. M. Lifshitz [1], in which the principle of minimization of the total free magnetic energy was proposed for the first time. The principles of micromagnetism are described in detail in the works of W.F. Brown (see, for example, [2]). At present, there are a large number of software packages, such as, for example, "OOMMF" [3], "mumax$^{(3)}$ "[4], and "Fidimag" [5], designed to solve an extensive class of micromagnetism problems [6].

The authors of this paper have previously developed two independent micromagnetic models: the model of single-domain particles with effective spontaneous magnetization (ODEN) [7, 8] and the model of two-phase chemically inhomogeneous particles (CHP) [9, 10], on the basis of which programs for micromagnetic modeling were created [11, 12]. These models have been successfully verified on various natural and artificial objects (see, for example, [13-19]. The main advantage of both models is the acceleration of calculations, since practically all computationally complicated expressions are calculated analytically in a general form [7, 9, 20].

In the present work, the object of micromagnetic modeling is zuvites, which are a type of rocks of impact origin resulting from a high-velocity impact of the Earth with a small space body. Unlike other impact rocks such as lithic breccias or impact glasses (see, for example, [21]), zuvites are polymict breccias containing a mixture of clastic material and fragments of molten target rocks (up to 10-15% or more) [22, 23, 17].

The Zhamanshin impact structure is located in the Northern Aral Sea region (Kazakhstan, 48.37°N, 60.94°E), with a pre-erosion diameter of ~ 13.5 km and an age of 0.91±0.14 Ma [24]. It was shown earlier that the Zhamanshin impactites (irgisites, zhamanshinites, tagamites, and zuvites) in geographically different parts of the crater differ in texture and chemical composition, which indicates that there was no global displacement of the target rocks during the impact event [25].

In [17], the magnetic properties of four samples of zuvites from the Zhamanshin impact structure were studied: three from the eastern part of the crater (samples ZSU-1, ZSU-2, and ZSU-3) and one from the northern part (sample 17-135). Theoretical calculations of hysteresis characteristics were carried out using the model of magnetostatically interacting single-domain particles with effective spontaneous magnetization. This allowed us to identify several features of the studied objects, including chemical heterogeneity and cluster distribution of iron oxide particles, and to show that the magnetic viscosity of zuwit samples is mainly provided by particles in the superparamagnetic state.

The purpose of the present work is the coordinated modeling of the hysteresis characteristics of the same zuvite samples based on the DF model and the modified ODEN model [26]. The coordinated modeling means theoretical calculation of the hysteresis characteristics of the samples by two independent models taking into account the experimental data: sample sizes and masses, saturation magnetization and residual saturation magnetization, coercivity and coercivity by residual magnetization, structural and phase composition.

THEORY AND EXPERIMENT

In [16, 27], the model of two-phase magnetostatically interacting particles was used to describe the magnetic states of chemically inhomogeneous particles. We considered an ensemble of cubic particles with characteristic size *a* and volumes of phases: $(1 - \varepsilon)a^{(3)\text{ - the}}$"strongly magnetic" phase and$\varepsilon a^{(3)\text{ - the}}$ "weakly magnetic" phase. The light magnetization axes of the phases were considered to be parallel to the interphase boundary. Then, in the absence of an external field, the magnetic moments in the phases are either opposite in direction or their directions coincide. Applying an external field parallel to the light axes does not increase the number of possible magnetic states, but changes their relative fractions. Within the framework of the DF model, it is possible to calculate the particle remagnetization fields and estimate the hysteresis characteristics of the sample in the approximation of a uniform distribution of random interaction fields.

Magnetostatic interaction even at small volume concentrations of ferrimagnetic (~1%) can significantly influence the magnetization processes [28]. This is all the more important in case of inhomogeneous (cluster) distribution of particles in the sample, when the concentration of particles in clusters can be much higher. In addition, the interaction leads to blocking of magnetic moments of a part of superparamagnetic particles, which can contribute to the residual magnetization (see, for example, [29]). Consequently, it is necessary to take into account the interaction parameters more strictly, for example, using the mean-field approximation for which the distribution functions of random fields are calculated [7].

By introducing the concept of effective spontaneous magnetization I_{eff}, which allows us to phenomenologically take into account the magnetic and chemical inhomogeneity of particles, we can consider the ensemble of conditionally "single-domain" magnetostatically interacting particles. In [14, 30], the authors of this article verified the ODEH model for an ensemble of synthesized particles of "magnetite-titanomagnetite" composition.

For magnetite-titanomagnetite composites, we performed coordinated calculations of hysteresis characteristics using both DF and ODEN models [31]. This allowed, on the one hand, to take into account the chemical inhomogeneity of individual particles and to calculate their remagnetization fields, and, on the other hand, to evaluate more strictly the influence of magnetostatic interaction between particles on the magnetization processes. Applying a similar approach using the modified ODEN model, we calculate the hysteresis characteristics of zuvinite samples.

Experimental data for the considered samples include [24]: 1) values of specific saturation magnetic moment M_s, residual specific saturation moment M_{rs}, coercivity $H_c$and coercivity by residual magnetization H_{cr}, obtained at room temperature on a LakeShore 7410 vibrating magnetometer (Lake Shore Cryotronics Inc, (Table 1); 2) values of magnetic susceptibility χ at three operating frequencies (976, 3904, and 15616 Hz) measured using the susceptibility bridge MFK-1FA (AGICO, Czech Republic).

It is known that the presence of the frequency dependence of the magnetic susceptibility χ indicates the presence of superparamagnetic particles in the samples and allows us to estimate the maximum possible values of the fraction of these particles (see, for example, [32, 33]). Using the values of magnetic susceptibility at the upper χ_h and lower frequencies χ_l in a weak field, it is possible to calculate the value of the FD factor (Frequency Dependence), the value of which *fd* (Table 1) correlates with the fraction of superparamagnetic particles in the ferrimagnetic fraction of the sample [15, 34]:

$$fd = \frac{\chi_l - \chi_h}{\chi_l \lg(f_h/f_l)} \cdot 100\%. \quad (1)$$

The values of the magnetogranulometric ratios M_{rs}/M_s and H_{cr}/H_c show that the particles are mainly in the single- and low-domain state [35]. At the same time, the value of the FD-factor shows that the fraction corresponding to truly superparamagnetic particles is present in the samples.

In the ODEN model, using the lognormal distribution of particles by volume [35, 36] and specifying ranges of particle sizes in different magnetic states [15], the fractions and average particle sizes in the selected ranges can be calculated. The probability density of the lognormal distribution is written as:

$$\varphi(x) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left(-\frac{(\ln(x/\alpha))^2}{2\sigma^2}\right), \quad (2)$$

where $x = v/v_p$ is the ratio of the particle volume to the mean volume, σ is the standard deviation and α is the mean of the corresponding Gaussian distribution. Five grain size ranges corresponding to different magnetic states are considered in the simulations: true superparamagnetic (SP), blocked superparamagnetic (bSP), single-domain (SD), pseudo-single-domain (PSD) and multi-domain (MD) particles with corresponding particle diameters approximately in the intervals 0-18, 18-25, 25-40, 40-100 and 100-

500 nm. The maximum possible content of particles in the true superparamagnetic state ranges from a few to tens of percent (see the value of *fd* in Table 1)

Let us introduce the relative fractions of particles corresponding to the above magnetic states: $n_{(sp)}$, n_{bsp} n_{sd}, n_{psd} and n_{md}. The relative fraction of each group is written as:

$$n = \int_{x_1}^{x_2} \varphi(x)dx / \int_{x_{min}}^{x_{max}} \varphi(x)dx, \quad (3)$$

where x_1 and x_2 are the lower and upper limits of the volume range of a given group of particles, respectively, $x_{(min)}$ ($d = 0$) and $x_{(max)}$ ($d = 500$ nm) are the minimum and maximum relative volumes of particles, respectively. Table 2 shows the relative contributions of particles in different magnetic states to the volume concentration of the sample ferrimagnetic corresponding to different possible values of the FD-factor and, consequently, different average values of the particle size d_{mean}. The best agreement with the experimental data was obtained for a characteristic particle size d_p= 25 nm (corresponding to the dimensionless mathematical expectation $M =$ 1) and a rather narrow distribution with a dimensionless standard deviation equal to 3.

Using the results of Table 2, coordinated calculations were performed for the two models of DF and ODEN. Based on the experimental values of M_s and M_{rs} and the assumed particle composition, the ODEN model sets a preliminary range of values of the effective spontaneous saturation magnetization $I_{(s)\ (eff)}$ and calculates the ferrimagnetic volume concentration C_f and the effective spontaneous magnetization $I_{(rs)\ (eff)}$ by the residual magnetization, taking into account the maximum value of the FD factor for each sample. And in the FD model, the remagnetization fields $H_{(0)\ \text{of}}$ particles of the same composition are calculated, corresponding to the experimental values of the coercivity by residual magnetization H_{cr}, which allows us to relate the value of *fd* to the oxidation degree ε through the average particle size $d_{(}$mean) . In both models, the particles are assumed to be crystallographically uniaxial, i.e., $H_0 = 2K_{(u)}/I_s$, where $K_u$is the effective constant of crystallographic anisotropy and $I_s$is the spontaneous magnetization of the particle (phase).

Table 3 shows the results of modeling corresponding to the assumed composition of two-phase particles of "magnetite/maghemite-hematite" type.

Comparative analysis of the obtained values of $I_{(s)\ (eff)}$and $I_{(rs)\ (eff)\ (}$Table 3) taking into account the approximation $H_0 = H_{cr}$and the corresponding values of spontaneous magnetizations and anisotropy constants of magnetite (I_s= 480 eme/cm^3, K_u= 1.3· 10^{5}erg/cm$^{3)}$, maghemite (I_s= 390 eme/cm$^{(3)}$·K_u= 4.6· 10^{4}erg/cm$^{(3}$)) and hematite (I_s= 3 eme/cm$^{(3)}$, K_u= 4· 10^{4}erg/cm^3) [37, 38] allows us to draw conclusions about the probable chemical composition and magnetic state of the particles. Samples ZSU-1 and ZSU-3 contain particles closer to the composition of "maghemite-hematite", and samples ZSU-2 and 17-135 - "magnetite-hematite". In all samples, the main contribution to the magnetic properties is made by single-domain and pseudo-single-domain chemically inhomogeneous particles. The most noticeable fraction of superparamagnetic particles is present in sample ZSU-2 (about 25-35%), which is manifested in a significant underestimation of the average particle size (see Tables 2 and 3). The volume concentration of ferrimagnetic in the samples is of the order of 10^{-3}-10^{-2}, and the concentration of superparamagnetic fraction is in the range of 10^{-5}-10$^{(-4)}$ $^{(}$see Table 3).

CONCLUSION

Thus, we have performed a coordinated theoretical modeling of the hysteresis characteristics of zuvites of the impact crater Zhamanshin on the basis of two independent micromagnetic models that take into account the possible chemical and magnetic heterogeneity of particles, as well as the magnetostatic interaction between them. The calculation results are in good agreement with the experimental data.

The approach using the frequency dependence of magnetic susceptibility allows us to estimate the concentrations of the superparamagnetic fraction in the samples corresponding to the values of the FD-factor. Although the volume concentration of superparamagnetic particles in the samples is small (of the order of 10^{-5}-$10^{-4)}$, but its consideration in modeling makes it possible to establish the parameters of the lognormal distribution of particles by volume and the assumed distribution of particles by magnetic states.

The comparative analysis of the obtained values of effective spontaneous magnetizations and remagnetization fields allowed us to draw conclusions about the chemical composition (magnetite-hematite, maghemite-hematite) and magnetic state of the particles (predominantly single-domain and pseudo-single-domain), as well as to determine the volume concentrations of ferrimagnetite in the samples.

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Table 1. Hysteresis characteristics and FD-factor values of the samples

Sample	M_s, eme/g	M_{rs}, eme/g	H_c, E	H_{cr}, E	M_{rs}/M_s	H_{cr}/H_c	*fd, %*
ZSU-1	0.71	0.11	139	318	0.16	2.3	10
ZSU-2	1.64	0.43	221	409	0.26	1.8	23
ZSU3	1.98	0.39	124	243	0.19	2.0	1
17-135	1.39	0.42	349	657	0.31	1.9	5

Table 2. Calculations of volume *fractions C* and mean sizes d_{mean}, corresponding to values of *fd* in the range from 0.5 to 23% (C_{SP} = *fd*), where *M* is the mathematical expectation of the lognormal distribution

M	2.61	2.31	1.95	1.37	0.79	0.14	0.06

C_{SP}, %	0.5	1.0	2.0	5.0	10.0	20.0	23.0
$C_{(b)\ (SP)}$, %	6.1	8.1	10.3	13.4	14.7	12.9	11.9
C_{SD}, %	44.7	44.1	42.5	38.1	32.0	22.2	19.6
C_{PSD}, %	48.6	46.6	44.7	42.3	40.0	34.2	31.8
C_{MD}, %	0.1	0.2	0.4	1.3	3.4	10.8	13.6
d_{mean}, nm	34	33	31	28	23	13	10

Table 3. Results of calculation of effective spontaneous saturation magnetization $I_{(s)\ (eff)}$, effective spontaneous magnetization $I_{(rs)\ (eff)}$by residual magnetization and volume concentration of ferrimagnetic $C_f$in the sample by two models. The lines with the best agreement by the two models are highlighted

Sample	Model	*fd* / ε	$I_{s\ eff}$, eme/cm^3	$I_{rs\ eff}$, eme/cm^3	C_f, 10^{-3}
ZSU-1	ODEN	2-10%	200	33-36	5.6
			300	49-54	3.7
			400	66-72	2.8
	DF	0,35-0,45	206-248	38-42	4.5-5.5
ZSU-2	ODEN	7-23%	200	59-71	12.5

			300	88-106	8.3
			400	117-142	6.2
	DF	0,01-0,35	312-475	114-152	5.3-8.0
ZSU-3	ODEN	0,1-1%	200	40	15.4
			300	60	10.3
			400	80-81	7.7
	DF	0,01-0,13	331-376	69-77	8.2-9.3
17-135	ODEN	1-5%	200	63-66	11.8
			300	95-99	7.8
			400	127-132	5.9
	DF	0,46-0,58	203-260	69-85	9.1-11.6