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Alignment of magnetic uniaxial particles in a magnetic field: Simulation

O.A. Golovnia [a,*], A.G Popov [a], A.N. Sobolev [b], G.C. Hadjipanayis [c]

[a] Institute of Metal Physics, Str. S. Kovalevskoy, 18, 620990 Ekaterinburg, Russia
[b] South Ural State University (National Research University), av. Lenina, 76, 454080 Chelyabinsk, Russia
[c] Department of Physics and Astronomy, University of Delaware, 217 Sharp Lab, Newark, DE 19716, USA

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ABSTRACT

The numerical investigations of the process of alignment of magnetically uniaxial Nd–Fe–B powders in an applied magnetic field were carried out using the discrete element method (DEM). It is shown that magnetic alignment of ensemble of spherical particles provides extremely high degree of alignment, which is achieved in low magnetic fields. A model of formation of anisotropic particles as a combination of spherical particles is suggested. The influence of the shape anisotropy and friction coefficient on the alignment degree was analyzed. The increase in the friction coefficient leads to a decrease in the alignment degree; the simulation results are in qualitative agreement with experimental dependences. It is shown that in magnetic fields higher than 5 T, the calculated field dependences of the alignment degree quantitatively render the experimental data. The increase of about 6% in the alignment degree in the experiments with addition of internal lubricant can be explained by the decrease of 14% in friction coefficient.

1. Introduction

One of the main tasks facing the manufacture of sintered magnets by means of powder-metallurgy method is magnetic alignment. A lot of parameters, such as magnetic properties of powder, geometry and shape of particles, filling density, strength and type of the applied magnetic field, etc., have to be optimized to achieve a high degree of alignment. The development of a new technology of producing sintered Nd–Fe–B permanent magnets, which is characterized by the absence of the stage of pressing powders (pressless process—PLP) [1–5], places higher demands on the process of magnetic alignment of the powder. It has been shown in [4] that increase in the filling density ρ_f of a powder placed in containers for sintering favors reaching a density of sintered magnet near the full density of cast alloy. However, increasing ρ_f leads to a sharp decrease in the degree of magnetic alignment of powders and, consequently, to a low remanence, B_r, of sintered magnets. The factor responsible for the decrease in the degree of alignment at $\rho_f \geq 3$ g/cm^3 is the friction forces between the powder particles. In this case, the degree of alignment can be increased by the application of a pulsed magnetic field of a high strength (higher than 8 T) or by the reduction of the friction forces via addition of internal lubricants, e.g. zinc stearate [5].

Simulation of the magnetic alignment of uniaxial magnetic powders should serve to reduce experimental trials and favor the understanding of the processes. In literature there are works on numerical investigations of the influence of type of powder compaction on the degree of the magnetic alignment achieved [6]. It has been shown that any type of compaction, both isostatic, with powders placed in an elastic matrix, and with the use of metal dies, in which the compaction direction is either parallel or transverse to the applied magnetic field, reduces the degree of magnetic alignment.

In view of extensive applications of the PLP technology, it is important to account for and understand in detail the effects of friction of the powder particles on their magnetic alignment.

The aim of the present work is to numerically simulate, using the discrete element method (DEM) [7], the process of magnetic alignment of uniaxial magnetic powders in the PLP technology. The method allows one to obtain dynamic information about the ensemble of particles, including their trajectories and velocities, the time-dependences of acting forces and torques, as well as other dynamic parameters, which eventually control the orientation of magnetic dipole moments of particles in the applied magnetic field. This information can hardly be provided by experimental procedures.

* Corresponding author. Tel.: +73433783782.
E-mail address: golovnya@imp.uran.ru (O.A. Golovnia).

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2. Mathematical model

In the model, a powder is an ensemble of ferromagnetic uniaxial particles with an average particle size d, mass m_i, and moment of inertia I_i. Each particle i experiences, along with the gravitational force $\mathbf{F}_i^g$, the contact force $\mathbf{F}_{ij}^c$ acting due to the interaction with a neighboring particle j and walls of the container and the non-contact force $\mathbf{F}_{ik}^{nc}$ caused by magnetostatic interaction. In addition, a torque $\mathbf{M}_{ij}$ acts on each particle. $\mathbf{F}_{ij}^c$ consists of the normal component $\mathbf{F}_n$ and tangential $\mathbf{F}_t$ component (Fig. 1). Thus, governing equations for translational and rotational motion of particles are written as

$$m_i\frac{d\mathbf{v}_i}{dt}=\sum_j\mathbf{F}_{ij}^c+\sum_k\mathbf{F}_{ik}^{nc}+\mathbf{F}_i^g, \tag{1}$$

$$I_i\frac{d\omega_i}{dt}=\sum_j\mathbf{M}_{ij}, \tag{2}$$

where $\mathbf{v}_i$ and ω_i are the translational and angular velocities of particle i. The force and torque caused by magnetostatic interaction between particles are written as

$$\mathbf{F}_{ik}^{nc}=1/(4\Pi\mu_0)(3((\mathbf{m}_i\cdot\mathbf{m}_k)\mathbf{r}+(\mathbf{m}_k\cdot\mathbf{r})\mathbf{m}_i+(\mathbf{m}_i\cdot\mathbf{r})\mathbf{m}_k)/r^5 -15(\mathbf{m}_i\cdot\mathbf{r})(\mathbf{m}_k\cdot\mathbf{r})\mathbf{r}/r^7) \tag{3}$$

$$\mathbf{M}_{ij}=1/(4\Pi\mu_0)(-(\mathbf{m}_i\times\mathbf{m}_j)/r^3+3(\mathbf{m}_j\cdot\mathbf{r})(\mathbf{m}_i\times\mathbf{r})/r^5), \tag{4}$$

where $\mathbf{m}_i$ is the magnetic dipole moment of particle i [8]. The torque caused by interaction with the applied magnetic field has the form

$$\mathbf{M}_i=\mathbf{m}_i\times\mathbf{H} \tag{5}$$

2.1. Contact forces

Generally, two particles contact each other through a finite area rather than a single point due to the deformation of the particles; this fact in the DEM is equivalent to the contact of two rigid bodies allowed to overlap slightly. Thus, the contact forces can be decomposed into a component in the contact plane $\mathbf{F}_t$ and one normal to the plane $\mathbf{F}_n$. Contact forces and torques are related to many geometrical and physical factors such as shape, material properties and state of motion of the particles [7].

For description of such complex interactions, the DEM generally adopts simplified models, e.g. non-linear spring-dashpot models based on Hertz model. The implemented modified Hertz model employs two non-linear springs: tangential and normal [8]. Thus, the contact force is given by

$$\mathbf{F}_{ij}^c=\sqrt{\delta}\sqrt{R_iR_j/(R_i+R_j)}[(k_n\delta\mathbf{n}_{ij}-m_{\mathrm{eff}}\gamma_n\mathbf{v}_n)-(k_t\Delta\mathbf{s}_t+m_{\mathrm{eff}}\gamma_t\mathbf{v}_t)], \tag{6}$$

where the first term is $\mathbf{F}_n$ and the second is $\mathbf{F}_t$ of contact forces; R_i is the radius of the spherical particle i; δ is the overlap distance of two particles; k_n and k_t are the elastic constants for the normal and tangential contact; γ_n and γ_t are the viscoelastic damping constants for the normal and tangential contact, respectively; $m_{\mathrm{eff}}=\mathbf{m}_i\mathbf{m}_j/(\mathbf{m}_i+\mathbf{m}_j)$ is the effective mass; $\Delta\mathbf{s}_t$ is the tangential displacement vector between two spherical particles; $\mathbf{n}_{ij}$ is a unit vector along the line connecting the centers of two particles; $\mathbf{v}_n$, $\mathbf{v}_t$ are the normal and tangential components of the relative velocity of two particles, respectively. In addition, the tangential force between two particles grows according to a tangential spring dashpot model until $\mathbf{F}_t=\mu\mathbf{F}_n$, where μ is the friction coefficient, $0<\mu<1$, which is valid until the particles lose contact [9–12].

3. Simulation details

The described method is implemented in the program software LAMMPS [13], i.e. Large-scale Atomic/Molecular Massively Parallel Simulator. For adaptation of the model to PLP experiments, it is divided into two stages. The first stage is creation of packing with the required filling powder density in the computational region which simulates a container for sintering. The rectangular container has a square base of side $10d$ and initial height of $200d$, where d is the diameter of a spherical particle. Its final height is calculated to fit the filling density. The particles are sparsely placed in the container with the initial height; afterwards they are packed by a moving lid until the filling density is achieved. The second stage is the alignment in a magnetic field, which achieves the set value of its strength instantaneously after the application. At this stage, the particles gain their magnetic dipole moments. In the model, we assume that the magnetization processes of the thermally demagnetized particles are finished before the magnetic alignment; therefore, orientation of the magnetic dipole moment of the spherical particles was chosen to make the projection of the magnetic dipole moment on the field direction vary in the range from 0 to$|\mathbf{m}|$. The magnetostatic interaction between the particles was computed within a sphere of the radius $2.5d$ and was cut off beyond it. The time step of calculations Δt was chosen in agreement with the standard approaches [14], so that the contact time of particles τ_{col} be no less than $50\Delta t$; Δt was actually equal to $\sim10^{-9}$ s at the first stage of simulation and $\sim10^{-11}$ s at the second stage.

For the estimation of the degree of alignment, the projection of magnetic dipole moment of the particles along the magnetic field direction, averaged over the ensemble, was employed. Thus, the degree of alignment was calculated as $\alpha_T=\cos\varphi$. In the experiment, the degree of alignment is usually defined as $\alpha_T=B_r/4\pi M_sV\alpha_\rho=B_r/B_s$, where $4\pi M_s$ is the saturation magnetization of the ferromagnetic phase of the alloy at room temperature; V is the volume fraction of the ferromagnetic phase in the magnet; α_ρ is the relative (with respect to the density of cast alloy) density of the sintered magnet; B_r is the remanence. The present work is devoted to the simulation of powders of the Nd–Fe–B alloy; calculation parameters are listed in Table 1 [6,15].

4. Results and discussion

4.1. Spherical particles

Fig. 2 shows time dependencies of the calculated degree of alignment achieved in applied magnetic fields of strength 0.1 to 1.4 T in an ensemble of 1000 spherical particles of diameter $d=1$ μm. According to the program algorithm, the particles were placed in the container, so that the final volume corresponds to a specified filling density of 3.4 g/cm^3 (or 45% of the density of the sintered magnet). However, balls dropped into the container form a denser packing (with the filling density about 60% of the density of the sintered magnet [16]). In this case, some free space, not occupied by the particles, exists under the lid. At the time $t=0$, the

Table 1
Calculation parameters.

Young's modulus of Nd–Fe–B, E	1.5×10^2 GPa
Elastic constants for normal contact k_n	$0.733E$
Elastic constants for tangential contact, k_t	$2/3k_n$
Viscoelastic damping constants for normal contact, γ_n	5×10^7 1/(s · m)
Viscoelastic damping constants for tangential contact, γ_t	$2/7\gamma_n$
Density of sintered Nd–Fe–B magnet, ρ	7.5 g/cm^3
Specific magnetization of Nd–Fe–B, σ	148.6 A · m^2/kg