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Numerical simulation of chainlike cluster movement of feeble magnetic particles by induced magnetic dipole moment under high magnetic fields

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Abstract
In this paper, the motion of a chainlike cluster of feeble magnetic particles induced by high magnetic field is discussed on the basis of the results of numerical simulations. The simulations were performed on glass particles with a diameter of 0.8 mm; and the viscosity, applied magnetic field and magnetic properties of the surrounding medium were changed. In addition to the magnetic field and the difference in magnetic susceptibility between the particles and the surrounding medium, the obtained results indicate that the viscosity is an essential factor for the formation of the chainlike alignment of feeble magnetic particles. We also carried out simulations using glass particles with a smaller diameter of 0.1 mm. Chainlike clusters were produced similar to those of ferromagnetic particles formed in a ferromagnetic fluid.

Keywords: magnetic field induced motion, feeble magnetic particles, chainlike clusters, alignment by magnetic field

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Much effort has been made to obtain one-dimensional structures of feeble magnetic materials, namely, diamagnetic and paramagnetic materials, under high magnetic fields. For example, needle-like fiber [1, 2], carbon nanotubes [3, 4] and inorganic crystals [5–7], which are typical one-dimensional materials, have attracted much interest because of their unique properties and potential applications in mechanical, electrical and thermodynamic devices. Chainlike materials are also considered one dimensional. For magnetic particles, the self-assembled chainlike structures formed by nano- and microparticles attract increasing interest because of their potential application in the fabrication of nano- and microdevices [8–11]. On the other hand, chainlike structures formed by feeble magnetic particles have received much less attention.

By the magneto-Archimedes effect [12], which is an increase in magnetic force by the surrounding environment, various effects of feeble magnetic materials have been
observed. In a series of studies using the magneto-Archimedes effect, magnetic dipole interactions have been observed among feeble magnetic particles that form a triangle-lattice structure at the air–liquid interface as well as among those that form a chainlike alignment and move while keeping their structure [13]. So far, we have paid attention to a two-dimensional triangle-lattice structure on a plane perpendicular to the direction of the applied magnetic fields, which is parallel to the direction of gravity. In our previous studies [14, 15], by experiment and numerical simulation, we examined and verified that the interaction among induced magnetic dipoles is a significant force that governs the structure formed by feeble magnetic substances under high magnetic fields.

In this paper, attention is given to the chainlike clusters of feeble magnetic particles. Movement of chainlike clusters is observed on a plane parallel to the applied magnetic field when the magnetic field is perpendicular to the direction of gravity. This is linked to the one-dimensional orientation of composite materials, inorganic crystals and polymers. First, a numerical simulation was performed by assuming experimental condition of the chainlike cluster movement. Then, in order to examine the factors controlling the chainlike alignment, we carried out numerical simulations varying the viscosity of medium, the strength of magnetic field, and differences in magnetic susceptibility between the particles and the medium. In addition, the potential of the chainlike structure formed by feeble magnetic particles is discussed by performing a simulation with particles having different diameters (0.8 mm and 0.1 mm). Through the above simulations, we discuss the chainlike structure of feeble magnetic particles that could have potential applications in various industrial fields, such as mechanical, electrical, medical and materials processing.

2. Physical conditions and experimental configurations

The experimental setup is shown in figure 1. The superconducting magnet was set horizontally. The sample particles were diamagnetic glass beads (diameter 0.8 mm). The medium in the magneto-Archimedes effect was manganese dichloride aqueous solution (MnCl2aq.) of 40 wt%. Table 1 shows the physical conditions for the experiment and numerical simulation. The glass beads and MnCl2aq. were put in a glass cell, and the cell was inserted into the bore of the magnet. One of the cell edges was fixed at the center of the fields, and the glass beads were gathered on that side initially. From this configuration, the magnetic field was gradually increased. Magnetic force acted on the glass beads which moved to the other side of the cell to distance themselves from the center of the field. These processes were observed from the bottom side of the cell with a charge coupled device (CCD) camera.

A photograph of the experimental results is shown in figure 2. As is evident in this figure, the glass beads formed chainlike structure parallel to the applied magnetic field as they moved away from the center of the magnetic field. In this figure, the magnetic field was applied from right to left, and its intensity at the center of the magnetic field was 2.5 T. The alignment originated from the attractive interactions among magnetic dipoles induced in the glass beads.

![Figure 1. Experimental setup.](image)

![Figure 2. Photograph of the experimental chainlike alignment of glass particles moving under a high magnetic field from left to right.](image)

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle (glass) Diameter</td>
<td>( d_p ) (mm)</td>
</tr>
<tr>
<td>Volume magnetic susceptibility</td>
<td>( \chi_p ) (−[SI])</td>
</tr>
<tr>
<td>Density</td>
<td>( \rho_p ) (g cm(^{-3}))</td>
</tr>
<tr>
<td>Medium (MnCl(_2)aq.) Concentration</td>
<td>( C ) (wt%)</td>
</tr>
<tr>
<td>Volume magnetic susceptibility</td>
<td>( \chi_f ) (−[SI])</td>
</tr>
<tr>
<td>Density</td>
<td>( \rho_f ) (g cm(^{-3}))</td>
</tr>
<tr>
<td>Viscosity</td>
<td>( \eta ) (mPa s)</td>
</tr>
</tbody>
</table>

*\( z = 0 \) is the center of the magnetic field, as shown in figure 1.

In this table, we summarized the physical conditions for the experiment and numerical simulation [13, 14].
3. Numerical simulation

3.1. Numerical model for the simulation

The objective of this study is to report the first attempt to examine the factors controlling the chainlike alignment of feeble magnetic particles. The main assumptions used in the numerical simulation are as follows:

- All particles are spherical and have the same diameter.
- The inertial force of an aqueous solution can be ignored because the Reynolds number of the particle is very small; in other words, the steady-state Stokes approximation is applicable.
- The change in magnetic field in particles can be ignored, and its value can be regarded as a magnetic field at the particle center because the particles are very small.
- Particles are sufficiently diluted in the medium; the hydrodynamic interactions among particles are ignored.
- The gravity, magneto-Archimedes levitation force and friction between the particles and the bottom of the cell are ignored.

We used the notation \( U_i^{(H)} \) for the potential energy of the interaction between particle \( i \) and the applied magnetic field, and the notation \( U_{ij}^{(m)} \) for the magnetic dipole interaction energy among particles \( i \) and \( j \). Thus, the expressions for these quantities are written as

\[
U_i^{(H)} = \frac{\pi d_p^3}{6} \left[ -\frac{1}{2\mu_0} (\chi_p - \chi_i) B_i^2 \right],
\]

and

\[
U_{ij}^{(m)} = \frac{\mu_i}{4\pi r_{ij}} \left[ (\mathbf{m}_i \cdot \mathbf{m}_j) - \frac{3}{r_{ij}^2} (\mathbf{m}_i \cdot \mathbf{r}_{ij}) (\mathbf{m}_j \cdot \mathbf{r}_{ij}) \right].
\]

Here, \( \chi_p \) and \( \chi_i \) are the volume magnetic susceptibilities of the particles and medium, respectively, and \( B_i \) is the magnetic flux density at the position of particle \( i \); \( d_p \) is the diameter of the particles, \( \mathbf{r}_i \) is the position of particle \( i \), \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \), \( r_{ij} = |\mathbf{r}_{ij}| \), and \( \mu_0 \) is the vacuum permeability. Because \( \chi_p \) and \( \chi_i \ll 1 \), we consider that \( \mathbf{H} \sim (1/\mu_0) \mathbf{B} \). The effective dipole moment \( \mathbf{m}_i \) in equation (1) denotes the induced magnetic dipole moment of diamagnetic particle \( i \) in a medium and is represented by the following equation [14, 15]:

\[
\mathbf{m}_i = \frac{\pi d_p^3}{2} \frac{\mu_p - \mu_i}{2\mu_i} \mathbf{H}_i.
\]

Here, \( \mu_p \) and \( \mu_i \) are the magnetic permeabilities of the particles and medium, respectively, and \( \mathbf{H}_i \) is the magnetic field at the position of particle \( i \).

Figure 3 shows the potential energy of the interaction between a magnetic field and a glass particle with a diameter of 0.8 mm. Figure 3(a) indicates the potential energy curves as a function of the \( z \)-position at \( r = 0 \), where \( r = 0 \) is the central axis of the bore of the magnet. The magnetic flux density at \( z = 0 \) and 80 mm are \( B = 2.5 \) and 2.1 T, respectively. The maximum magnetic flux density is obtained at \( z = 0 \). Figure 3(b) shows the potential energy curves as functions of the \( r \) position in three \( z \) positions. The potential energy for the \( r \)-direction is minimum at \( r = 0 \) mm. The energy curves in figure 3(b) indicate that a central force in the \( r \)-direction acts on glass particles.

3.2. Equations of motion

The motion of an arbitrary particle \( i \) in the model system is governed by the following equation, which is expressed in a nondimensional form. As reported in section 3.1, the simulation did not estimate the frictional force between the particles and the bottom of the cell.

\[
\frac{dv_i^r}{dr} = F_i^{(H)i} + \sum_{i \neq j} F_i^{(m)ij} - F_i^{(v)i}.
\]

Here \( F_i^{(H)i} \), \( F_i^{(m)ij} \) and \( F_i^{(v)i} \) are the magnetic force that the applied magnetic field exerts on particle \( i \), the magnetic interaction force between particles \( i \) and \( j \), and the viscous drag by the medium, respectively. These dimensionless forces are normalized by the representative force \( F_0^{(m)} \) [15].

3.3. Conditions and outline of the numerical simulation

In this study, the unit scale of the length is the diameter of the particle. The simulations of the particle motion were performed in a cell with a width of 40 and a length of 100. This translates into a width of 32 mm and a length of 80 mm, as the diameter of the particle is 0.8 mm. Initially, all 120 particles
are positioned within the width $z$ range of 0–5. The particle motion was then simulated using an MD method based on the velocity Verlet algorithm.

First, a simulation was performed by assuming experimental conditions. Subsequently, the dependence of particle alignment on the viscosity of the medium was examined by simulation by changing the viscosity. We then examined the effects of the formed structure by changing the magnetic environment. We considered two cases: the change in the intensity of the applied magnetic field, $B$, and the difference in magnetic susceptibility between the particles and the medium, $\Delta \chi = \chi_p - \chi_f$. In both cases, we assumed that their values are double, i.e. $2B$ and $2\Delta \chi$. Moreover, the behavior of particles was examined when their diameter was reduced to 0.1 mm.

4. Results and discussion

4.1. Simulation by assuming experimental conditions

The results of the numerical simulation performed by assuming the same conditions as those in the experiment are shown in figure 4. It was confirmed that glass particles with a diameter of 0.8 mm form a chainlike alignment, as observed in the experiment, by considering the interactions among the induced magnetic dipoles described in equation (4). In this simulation, it took about 7 s for all particles to reach the opposite side. In the actual experiment shown in figure 2, this took about 50 s. The difference is because we did not consider the friction between the particles and the underside of the cell, gravity, and the magneto-Archimedes levitation, as reported in the main assumptions in section 3.1. Therefore, in this paper, we treat the time in the figures as a reference value for the numerical simulation and compare the time ratios.

4.1.1 Dependence on the viscosity of fluid. Simulations were carried out by changing the viscosity of the medium. As shown in table 1, the viscosity $\eta_f$ of the 40 wt% MnCl$_2$ aqueous solution used in the experiment is 10 times that of water. In this study, to evaluate the effect of the viscosity of the medium, two viscosities, namely $0.1 \eta_f$ and $10 \eta_f$, are assumed without changing the magnetic susceptibility of the medium. Figures 5(a) and (b) show the results for $0.1 \eta_f$ and $10 \eta_f$, respectively. Here, three image data show the times when the head of the particle group reached $z = 10, 50$ and 100.

From figure 5, when the viscosity of the medium is $0.1 \eta_f$, that is, the same as the viscosity of water, it is evident that particles do not form a chainlike structure and each particle moves individually. This result shows that the viscosity of the medium is an important factor for the formation of the chainlike alignment of feeble magnetic particles by the induced magnetic dipole moment.

4.2. Dependence on the magnetic environment

The applied magnetic field $B$ and the difference in magnetic susceptibility $\Delta \chi$, are two very important factors for the formation of a chainlike alignment because it is formed by magnetic interactions among magnetic dipole moments. Here, the numerical simulation performed by changing the surrounding magnetic environment was carried out for two cases, $B$ and $\Delta \chi$. For both cases, the value used in the simulation is twice that used in the experiment. From equations (1) and (3), in this study, it is evident that $\Delta \chi$ is a more significant factor than its constituent magnetic susceptibility. Here, to obtain $2\Delta \chi$, only the magnetic susceptibility of the particles was changed, and not that of the surrounding medium.
Figure 5. Simulation results for various viscosities: (a) 0.1ηf and (b) 10ηf. The scale unit is the diameter of a particle, 0.8 mm.

Figure 6. Simulation results for changing surrounding conditions: (a) double the applied magnetic field (2B) and (b) double the difference in magnetic susceptibility (2Δχ). The scale unit is the diameter of a particle.

Figure 6(a) shows the result of doubling the intensity of magnetic flux density 2B, and (b) shows the result of doubling the difference in magnetic susceptibility 2Δχ. When the applied magnetic field is doubled, there are no significant differences from the result obtained in figure 4, except that the travel time of the particles decreases. This result is caused by synchronous changes in two magnetic forces acting on the particles, which are the dipole interaction and the magnetic force, because U^{(HF)} and U^{(m)} are both second-order functions of B. However, this does not mean that the formation of a particle alignment does not depend on the intensity of the magnetic field. This simulation did not consider the friction between the particles and the base of the cell. Indeed, when the magnetic force is smaller than the friction, particles have difficulty in moving and do not form a chainlike alignment. On the other hand, when the difference in magnetic susceptibility is doubled, as shown in figure 6(b), chainlike lines move with a highly aggregated group in contact with each other. In this
Figure 7. Simulation results for particle diameter \( d_p = 0.1 \text{ mm} \); the scale unit is the particle diameter.

In this case, \( U^{(H)} \) is a first-order function of \( \Delta \chi \), and \( U^{(m)} \) is a second-order function of \( \Delta \chi \), because \( m_i \) of equation (3) is a function of the difference in magnetic susceptibility \( \Delta \chi \).

We examined the results of simulations performed by changing the viscosity of medium while changing the surrounding magnetic environment. These results are shown in appendix A. In both results, there are no significant differences in particle alignment at different viscosities, and the results are similar to those in figure 5.

4.3. Simulation for smaller particles

A numerical simulation for a smaller particle, \( d_p = 0.1 \text{ mm} \), was carried out and the results are shown in figure 7. In this case, the particles are initially randomly located in the area of \( 40d_p \times 40d_p \). As shown in figure 7, particles initially move to align in the direction of the applied magnetic field rather than going forward. After many chainlike lines are formed, they begin to move away from the center of the magnetic field. Although time is relative in these figures, chainlike lines take about 20 s to move for the length of \( 10d_p = 1 \text{ mm} \). From figure 3(a), it is found that the magnetic force, namely, the gradient of potential \( U^{(H)} \), is very small at the central area used in this simulation. The chainlike alignments obtained in this simulation are very long just as ferromagnetic particles in a ferrofluid form chainlike clusters, as determined by numerical simulation with a uniform magnetic field [16]. As discussed in section 4.1.1, we expected to control the cluster speed by selecting media with various viscosities.

Figure A.1. Simulation results for various viscosities \( \eta_f \) on doubling the applied magnetic field \((2B)\): (a) 0.1\( \eta_f \) and (b) 10\( \eta_f \). The scale unit is the diameter of a particle, 0.8 mm.

5. Conclusion

The chainlike cluster movement of feeble magnetic particles with a diameter of 0.8 mm observed in an experiment, whose plane is parallel to magnetic field and perpendicular to gravity, was studied by numerical simulations. We examined the results of simulations performed by changing the viscosity of medium and found that particles do not form a chainlike alignment and each particle moves individually when the
The viscosity of the medium is low. This result indicates that the viscosity of the medium is an important factor for the formation of the chainlike alignment of feeble magnetic particles by the induced magnetic dipole moment, in addition to the magnetic field and the magnetism of the surrounding medium. Furthermore, numerical simulations were carried out for changing the surrounding magnetic environmental conditions—the applied magnetic field $B$ and difference of magnetic susceptibility $\Delta \chi$. In both cases, their values are twice higher than those in the experiment. For the former, no significant differences in formation characteristics were observed. On the other hand, for the latter, a difference in the degree of aggregation was observed. Moreover, we carried out a numerical simulation using a smaller particle with a diameter of 0.1 mm. Very long chainlike clusters are formed in this case, similar to those of ferromagnetic particles in a ferrofluid. We anticipate that we could control the cluster speed by choosing media with various viscosities. Specifically, we believe that using media with high viscosities would result in the delay of the travelling of a chainlike cluster. The results presented in this paper lead to interesting suggestions about the applications of feeble magnetic particles to the device fabrication. In the future, in order to evaluate the obtained alignments, a precise numerical simulation should be performed by considering the friction of a particle and the underside of a cell and the magneto-Archimedes levitation. The chainlike structure formed by feeble magnetic particles could have potential applications to the formation of a one-dimensional structure in various industrial fields, such as mechanical, electrical, medical and materials processing.

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Appendix. Comparison of change in viscosity with change in surrounding magnetic environment

We examined simulations by changing the viscosity of medium to change the surrounding magnetic environment, which is discussed in section 4.2. Figure A.1 shows the result of doubling the applied magnetic field $2B$, and figure A.2 shows the result of doubling the magnetic susceptibility $2\Delta \chi$. Similarly to section 4.1.1, the viscosities of the medium examined in these numerical simulations are 0.1 and 10 times $\eta_f$.

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