J. Phys. D: Appl. Phys., 13 (1980) L119–22. Printed in Great Britain

LETTER TO THE EDITOR

Particle cluster configuration in magnetic fluids

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Received 18 April 1980

Abstract. A model based on Monte Carlo methods has been used to investigate the effects of magnetostatic and repulsive interparticle interactions on the properties of a magnetic fluid. The model predicts the formation of open loop structures in the absence of a magnetic field, and long chains in the presence of large magnetic fields. The model also predicts that the initial susceptibility is reduced in the presence of interactions. These predictions are in agreement with experimental observations.

Magnetostatic interparticle interactions play an important role in determining the magnetic properties and stability of a magnetic fluid. This paper presents the initial results of a calculation of the effect of magnetostatic interactions on the properties of a magnetic fluid. The calculation is based on Monte Carlo methods and is used to predict the configurations which the particles of a magnetic fluid take up due to interactions, and how the configurations vary with the magnetic field strength.

Consider a two dimensional system of N spherical particles of diameter D in a square with side of length A. The position of any particle can be specified by the coordinates (x, y, θ) where θ is the angle between the magnetic moment of the particle and the applied magnetic field H. The energy, E_i, of particle i, consists of three contributions

$$E_i = E_m + E_r + E_h. \tag{1}$$

E_m is the magnetostatic interaction energy

$$E_m = -\sum_{j \neq 1} (I'^2_s \pi^2 D^6 / 36 R_{ij}^3) [2 \cos(\theta_i - \psi) \cos(\theta_j - \psi) - \sin(\theta_i - \psi) \sin(\theta_j - \psi)]. \tag{2}$$

I'_s is the saturation magnetisation of the bulk material, and R_{ij} is the centre to centre distance between particles i and j. θ_i and θ_j are the angles between the magnetic moment and the applied field for particles i and j respectively, and ψ is the angle between the magnetic field and the line joining the centre of the particles.

E_r is the energy due to the repulsive force between the particles caused by the surfactant coating which is a necessary requirement for the magnetic fluid to retain long term stability. Rosensweig *et al* (1965) have shown that E_r is given by

$$E_r = \frac{\pi D^2 N'}{4} \left(2 - \frac{(h+2)}{b} \ln \frac{(1+b)}{(1+h/2)} - \frac{h}{b}\right) \tag{3}$$

0022-3727/80/070119+04 $01.50

where $h=(2R_{ij}/D-2)$, $b=2\delta/D$, and δ is the thickness of the surfactant coating. N' is the number of surfactant molecules/unit area of the particle surface. Equation (3) is applicable when $R_{ij} \leqslant (D+2\delta)$. For $R_{ij} > (D+2\delta)$, $E_r=0$. E_h, the energy of the particle in a magnetic field, is given by

$$E_h = -\mu H \cos \theta_i \tag{4}$$

where $\mu=\pi I'_s D^3/6$ is the magnetic moment of the particle.

The method used here is based on that first proposed by Metropolis *et al* (1953). The energy E_i of particle i with coordinates (x_i, y_i, θ_i) is calculated using equations (1)–(4), where E_m is calculated for interactions with $R_{ij} < 5D$. The particle is then moved at random to new coordinates (x'_i, y'_i, θ'_i), and the energy E'_i of the particle in its new position is calculated. If the energy difference $\Delta E = E'_i - E_i$ is negative, the move is allowed, and the particle retains the new coordinates. If ΔE is positive, a random number $X(0 \leqslant X \leqslant 1)$ is generated and compared with $\exp(-\Delta R/kT)$. If $\exp(-\Delta E/kT) > X$, the move is allowed. However, if $X > \exp(-\Delta E/kT)$, the move is disallowed and the particle is returned to its original position.

This procedure is carried out for all of the N particles in turn, and is repeated for the whole system until the magnetism converges to an essentially constant value. After a sufficiently large number of moves, the configuration is a typical picture of the system in thermal equilibrium.

The reduced magnetisation of the system, $\bar{I}=I(H)/I_s$, where $I(H)$ and I_s are the magnetisations of the system in a field H and at saturation respectively, is given by

$$\bar{I} = \text{Lim}\left(\sum_{k=1}^{n} (\cos \theta_k)/n\right) \tag{5}$$

where θ_k is the value of θ at the end of move k, and n is the total number of moves.

The configurations and reduced magnetisation have been calculated for cobalt particles ($I'_s = 1400$ emu cm^{-3}) of 150 Å diameter, for various values of the applied field H. Figure 1 shows the thermal equilibrium configuration in zero applied field, and figure 2 shows the configuration for an applied field of 10 kOe.

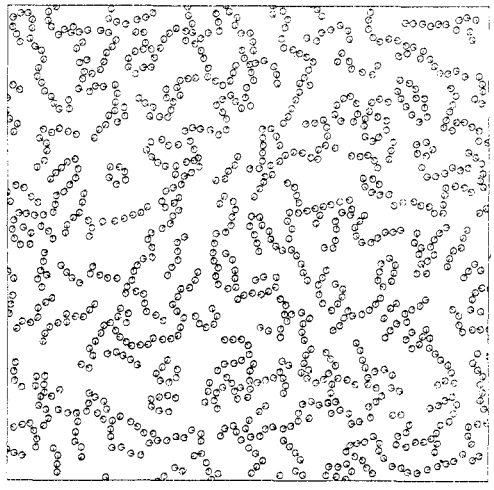

Figure 1. 150 Å diameter Co particles in zero field.

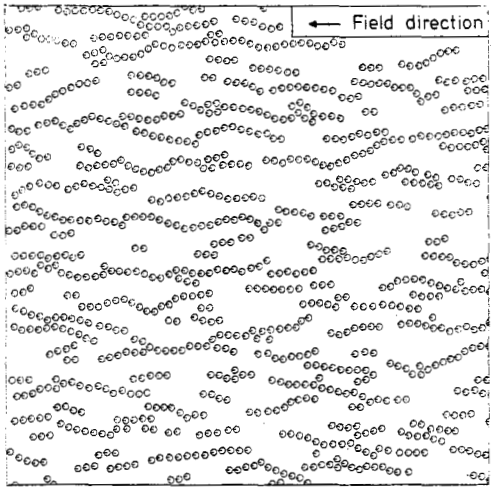

Figure 2. 150 Å diameter Co particles in an applied magnetic field of 10 kOe.

In zero applied field, the particles form open loop structures with no particular spatial orientation. In a large applied field of 10 kOe, the particles form long chains which are oriented along the applied field direction. These results are consistent with experimental data (Hess and Parker 1966, Martinet 1974).

Figure 3 shows the theoretical magnetisation curve (A) for 150 Å cobalt particles. Also shown is the magnetisation curve (B) for particles assumed to be non-interacting. It can be seen that the effect of interactions reduces the initial susceptibility of the system.

The two-dimensional model successfully predicts the observed phenomenon of open loop structure for particles in zero field which break up into chains of increasing length under the influence of an applied field of increasing magnitude.

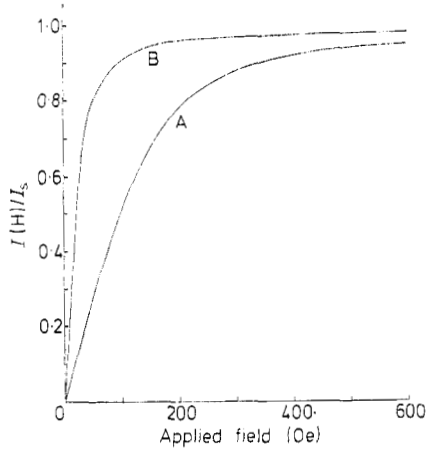

Figure 3. Reduced magnetisation curves for 150 Å diameter Co particles. Curve B, non-interacting particles; curve A, particles with magnetic interactions. 20 Å coating thickness.

Further experimental and theoretical work is at present being carried out in order to make a comparison between experimental and theoretical magnetisation curves. In order to compare experimental and theoretical configurations, it is necessary to devise a method of assessing the effect of interactions on the configuration. A method of analysis based on the radial distribution function has given encouraging initial results.

Consideration is also being given to extending the calculations to a three-dimensional system containing a distribution of particle size.

References

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