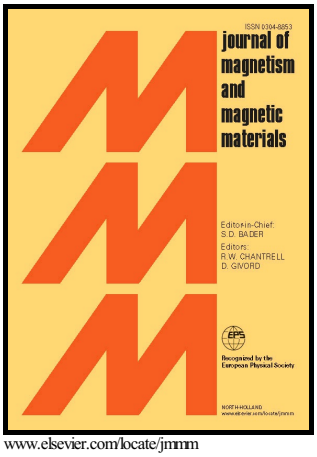

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Cluster Analysis in Systems of Magnetic Spheres and Cubes

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Abstract

In the present work we use molecular dynamics simulations and graph-theory based cluster analysis to compare self-assembly in systems of magnetic spheres, and cubes where the dipole moment is oriented along the side of the cube in the [001] crystallographic direction. We show that under same conditions cubes aggregate far less than their spherical counterparts. This difference can be explained in terms of the volume of phase space in which the formation of the bond is thermodynamically advantageous. It follows that this volume is much larger for a dipolar sphere than for a dipolar cube.

Keywords: magnetic colloids, self-assembly, computer simulations, cluster analysis

1. Introduction

In the last decades, as a result of rapid advances in synthesis techniques, a new branch of science has emerged – dipolar soft matter. This new field is concerned with the study of magnetic nano/mirco-particles, which nowadays can be synthesised in a variety of shapes: cubes [1, 2, 3, 4, 5], ellipsoids or rods, [6, 7, 8] and many others. One can safely state that the colloidal anisometry can be used as an effective control parameter to tune self-assembly scenarios as well as the thermodynamic, rheological and phase behaviour of dipolar soft matter [9].

In addition to making the particle shape anisometric, one can create Janus-like particles [10, 11] or patchy colloids [12, 13]. Magnetic janus particles are usually comprised of one magnetic and one non-magnetic hemisphere[10, 14, 15, 16, 17, 18, 19], where up to now only a few theoretical models are known that aim at predicting the behaviour of these particles[20, 21]. A variation on the theme is achieved when one uses silica particles partially covered with a ferromagnetic thin film to form capped magnetic colloids.[22, 23, 24, 25, 26].

The progress and flexibility of colloidal design in recent years is revealing potential new applications of magnetic soft matter in biomedicine: sensors, contrast agents, drug targeting, hyperthermia cancer-treatment therapy, cell manipulation are some important examples [27, 28, 29, 30]. Behind each application there is a need for a fundamental understanding of the relationship between the shape and structure of the magnetic colloids, the properties of the carrier matrix, and how they both relate to the macroscopic response of the complete material.

In our systems of magnetic spheres and cubes the dominant interaction is the classical long-range anisotropic magnetic dipole-dipole interaction. The interaction between cubes is still dipolar, as we assume, that inside a nonmagnetic cube there is a magnetic nanoparticle of a spherical shape. On the level of two particles with dipole moments $\boldsymbol{\mu}_i$ at positions $\mathbf{r}_i$ it can be written as:

$$U_{dd}(ij) = -3\frac{(\boldsymbol{\mu}_i \cdot \mathbf{r}_{ij})(\boldsymbol{\mu}_j \cdot \mathbf{r}_{ij})}{r^5} + \frac{(\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j)}{r^3}, \qquad (1)$$

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \quad |\mathbf{r}_{ij}| = r.$$

This potential depends not only upon the inter-particle distance r, but also on the mutual orientation of the particles' magnetic moments. It is convenient to introduce the dipolar coupling parameter $\lambda = \mu^2/k_{\mathrm{B}}T\sigma^3$, which denotes the ratio of the magnetic interaction energy per particle of two perfectly co-aligned dipoles at close contact σ relative to thermal energy $k_{\mathrm{B}}T$. Neighbouring particles, due to their dipolar interactions, favour a head-to-tail configuration. It follows, when this interaction becomes stronger than the thermal fluctuations of the system, a directed self-assembly of the particles is observed.[31, 32, 33, 34, 35, 36]. In order to allow for the presence of excluded volume in the system one needs a steric potential to prevent particle overlap. In this work, we have utilised a soft core interaction between the nanoparticles given by the Weeks-Chandler-Andersen pair potential [37]:

$$U_{\mathrm{WCA}}(r) = \begin{cases} U_{\mathrm{LJ}}(r) - U_{\mathrm{LJ}}(r_{cut}), & r < r_{\mathrm{cut}} \\ 0, & r \geq r_{\mathrm{cut}} \end{cases}, \qquad (2)$$

where $U_{\mathrm{LJ}}(r)$ is the Lennard-Jones potential:

$$U_{\mathrm{LJ}}(r) = 4\epsilon_s[(\sigma/r)^{12} - (\sigma/r)^6], \qquad (3)$$

which within expression (2) has been truncated at the position of its minimum and shifted by the corresponding depth to make the resulting potential purely repulsive. The parameter ϵ_s sets the energy scale in the system.

Based on these two interactions, we have analysed the self-assembly occurring in systems of dipolar soft spheres and dipolar soft cubes. In the next section we describe the methodology. Thereafter, we present the results and a comparison of the two systems, finishing with a brief summary in the conclusions.

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