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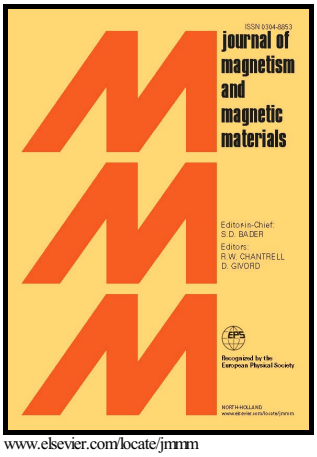

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Self-Diffusion in Monodisperse Three-Dimensional Magnetic Fluids by Molecular Dynamics Simulations

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Abstract

In the present work we study the self-diffusion behaviour in the three-dimensional monodisperse magnetic fluids using the Molecular Dynamics Simulation and Density Functional Theory. The peculiarity of computer simulation is to study two different systems: dipolar and soft sphere ones. In the theoretical method, it is important to choose the approximation for the main structures, which are chains. We compare the theoretical results and the computer simulation data for the self-diffusion coefficient as a function of the particle volume fraction and magnetic dipole-dipole interaction parameter and find the qualitative and quantitative agreement to be good.

Keywords: self-diffusion, magnetic fluids, chain aggregates, molecular dynamics simulations, density functional theory

1. Introduction

Magnetic fluids are the systems consisting of single-domain magnetic nanoparticles suspended in a carrier liquid [1, 2, 3]. An unique combination to interact with an external magnetic field and to be a liquid presents the basis for practical application of magnetic fluids. They are used for development of new technologies, creation of new constructions of machines and devices [4]. Medical applications of ferrofluids are the most important and perspective ones. For example, magnetic fluids are used for magnetic drug targeting [5], magnetic resonance imaging [6], and hyperthermia cancer-treatment therapy [5, 7].

Magnetic nanoparticles have intrinsic magnetic moments. The main interaction between ferromagnetic particles is a magnetic dipole-dipole interaction. The minimum of this potential is a "head-to-tail" orientation of magnetic moments. If the interactions in the system are strong enough the structures like chain aggregates are likely to form. So, the system under the theoretical study consists of chain aggregates. Of course, there are several works dealing with the study of diffusion behaviour in magnetic fluids [8, 9, 10, 11, 12]. The main difference of these papers from the present work is a study of the gradient diffusion in ferrofluids. Also note that ferrofluids with microstructure are not taken into account in the majority of works [8, 9, 10, 11]. Rigid chain aggregates consisting of ferromagnetic particles were considered in the work [12] as a microstructure. In the present paper, we consider flexible chains of magnetic particles.

The paper is organised as follows. Firstly (Section 2), we discuss the basic model for the study and the main methods of investigation. In the next section (Section 3), we compare the computer simulation data and theoretical results. Conclusion contains the summary and outlook.

2. Model and Methods

2.1. Model

We consider the three-dimensional monodisperse ferrofluids. The main interaction between magnetic nanoparticles can be described by the magnetic dipole-dipole potential [13]:

$$U_{dd}(i,j) = \frac{\mu_0}{4\pi}\left(\frac{\langle \vec{m}_i, \vec{m}_j\rangle}{|\vec{r}_{ij}|^3} - \frac{3}{|\vec{r}_{ij}|^5}\langle \vec{m}_i, \vec{r}_{ij}\rangle\langle \vec{m}_j, \vec{r}_{ij}\rangle\right), \quad (1)$$

where $\vec{m}_i$ and $\vec{m}_j$ are the magnetic moments of i^{th} and j^{th} magnetic particles, respectively; $\vec{r}_{ij}$ is the vector connecting the centres of i^{th} and j^{th} particles, $\mu_0 = 4\pi \times 10^{-7}$ H/m is the magnetic permeability of vacuum.

The interaction can be characterized by the parameter, which is the ratio of magnetic energy to the thermal one:

$$\lambda = \frac{\mu_0 \left|\vec{m}\right|^2}{4\pi k T d^3}, \quad (2)$$

where kT is the thermal energy, d is the diameter of particles.

A short-range repulsion between particles is described by the Weeks-Chandler-Andersen potential [14]:

$$U_{WCA}(i,j) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] + \varepsilon, & r \le r_c, \\ 0, & r > r_c. \end{cases} \quad (3)$$

where ε is the potential well depth, σ is a distance when the interaction energy becomes equal to zero.

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