3D Monte Carlo Simulations of Structural Regime Change in Magnetic Janus Particle Aggregates

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Magnetic particle suspensions have actively been studied in research fields such as fluid engineering, colloid and surface engineering, biomedical engineering and environmental resource engineering. In these applications, it is necessary to develop an accurate method for controlling the internal structure of particle aggregates using an external magnetic field. Recently, many researchers have focused on suspensions composed of spherical Janus particles whose hemispheres are covered by magnetic materials [1,2]. For magnetic Janus particles, it is predicted that the internal structure of their aggregates differs from that of conventional magnetic particles. From this background, in the present study, we investigated the transition of aggregate structures in a suspension of magnetic Janus particles under a uniform magnetic field. Three-dimensional Monte Carlo simulations were carried out in order to investigate the dependence of the transition of aggregate structures on various factors, such as the magnetic interaction between particles, an applied magnetic field and the distance between the magnetic moment and the particle centre. Here, we employ a particle model [2] in which the magnetic moment is radially shifted with respect to the particle centre. The main results obtained here are summarized as follows. For Janus particles whose magnetic moments are near their centre, long chain-like clusters tend to be formed in a system when the magnetic particle-particle interaction is sufficiently strong. In the case of strong magnetic interactions, an increase in the distance between the magnetic moment and the particle centre leads to a transition in aggregate structures from chain-like clusters to cluster units consisting of 2 to 5 particles. With increasing the strength of the magnetic field, chain-like clusters have a strong tendency to be formed aligned in the direction of an applied magnetic field. For Janus particles with magnetic moments near their surface, those in chain-like clusters tend to arrange so that their magnetic caps are close to each other. From these results, we demonstrate that the strength of magnetic interaction between particles, the applied magnetic field strength, and the position of the magnetic moment strongly influence the internal structure of particle aggregates and the orientation of magnetic caps in Janus particle assemblies. It may be important that these results provide valuable guidance for designing highly functional particle systems.

Keywords:
Magnetic Janus particle, Monte Carlo simulation, Aggregate structure, Uniform magnetic field, Thermodynamic equilibrium

References:

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