Monte Carlo simulations of aggregate-structure transitions of hexagonal plate-like hematite particles in a quasi-two-dimensional system

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Monte Carlo simulations were performed for a quasi-two-dimensional dispersion of hexagonal plate-like hematite particles to investigate aggregate-structure transitions and their internal structures. The analysis was limited to a quasi-two-dimensional model in which particle centers were confined to a plane, a single magnetic moment was fixed at the particle center, and Néel relaxation was not included. A hexagonal prism model was introduced with an explicit contact test for polyhedral particles, and two in-plane magnetization models were considered by assigning the magnetic moment along either the opposite-vertex direction or the opposite-edge-midpoint direction of the hexagonal plate. Without an external magnetic field (Fig.1 (a)), strong magnetic particle-particle interactions led to the formation of column-like clusters, where particle axes were aligned and neighboring magnetic moments tended to arrange in an antiparallel manner. Under a magnetic field applied perpendicular to the plane (Fig.1 (b)), these column-like clusters collapsed and the number of isolated particles increased. For particles with the same volume and material, increasing the aspect ratio shifted the onset of the rapid increase in the order parameters to weaker interaction conditions, indicating that particles with larger aspect ratios form aggregates more easily. This trend was almost independent of the magnetization model in the examined conditions. In addition, the parameter sweep (mainly for aspect ratios of 3 or larger) was chosen within a range where equilibration was practically achievable in the present MC framework. These results suggest that, within the present model assumptions and parameter range, aggregate-structure transitions are governed mainly by the magnetic interaction strength, the applied field strength, and the particle aspect ratio, rather than by the difference between the two magnetization models.

Keywords:
Hexagonal plate-like particle, Shape anisotropy, Magnetization model, Aggregate structures, Monte Carlo simulation

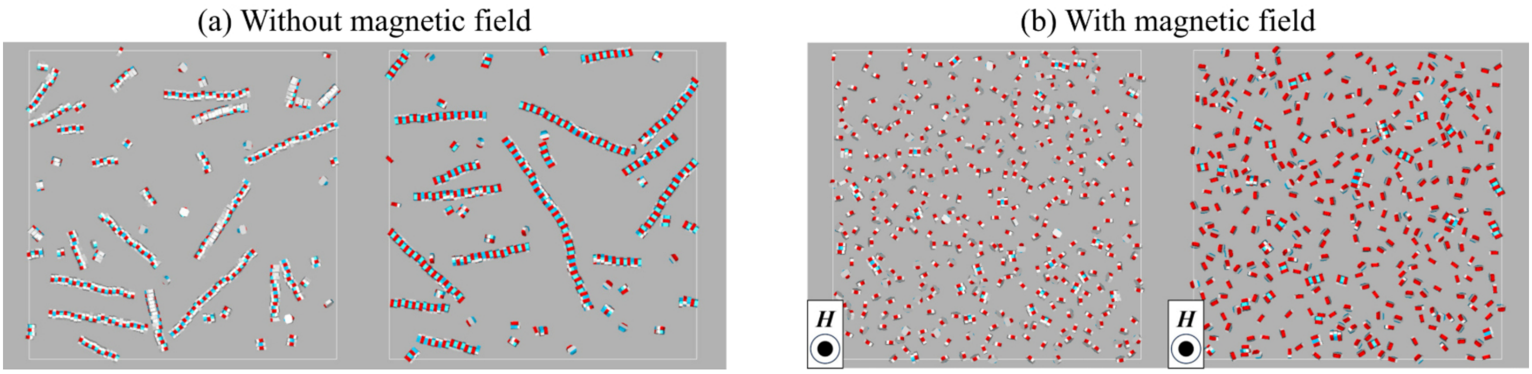

Fig.1 Aggregate-structure transitions of hexagonal plate-like hematite particles

Acknowledgements:
The authors would like to gratefully acknowledge the use of computational resources provided by the Centro de Supercomputación de Galicia (CESGA), Galicia, Spain.