Mesoscale Modeling of Colloidal Films Dried with Controlling the Morphology of Aggregated Particles

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Extended Abstract

Colloidal suspensions are coated on substrates and upon drying produce various functional films, whose quality is determined by the structure composed of colloidal particles. This structure can be controlled by the morphology of aggregated colloidal particles formed in host fluids. For example, network structure is suitable for transparent conductive composite films and porous materials such as thermal insulator. In the present study, we construct a mesoscale simulation model to investigate how the morphology of aggregated particles in host fluids affects the structure of dried colloidal films.

In our mesoscale simulation model[1-3], we describe the Brownian motion of spherical particles by a stochastic differential equation called the Langevin equation. We additionally construct a detailed model to describe adhesion between contacting particles by introducing a phenomenological constraint force and torque on the relative translational and rotational motion between the particles. This model enables us to consider the formation of various morphology of aggregated particles as shown in Fig. 1. The adhesion between particles results in the network structure formed by the connection of chain-like particle clusters. In real systems, the adhesion is considered to be given by adding binders.

We investigate the structure of the dried colloidal films depending on the morphology of aggregated particles. We model the evaporation process of host fluids by a receding free surface that exerts capillary forces on the particles. Figure 2 shows the formation of a particle network during drying calculated through the present model. The particles aggregate together into chain-like clusters by the adhesion. When the free surface approaches the substrate, the clusters overlap each other and partially aggregate by the capillary force to form a network structure. In terms of the properties of transparent conductive films, the connectivity and the coverage on the substrate of the network are reflected in the conductivity and the transparency, respectively. Using the present model, we propose how to control the structure of dried colloidal films by the morphology of aggregated particles.

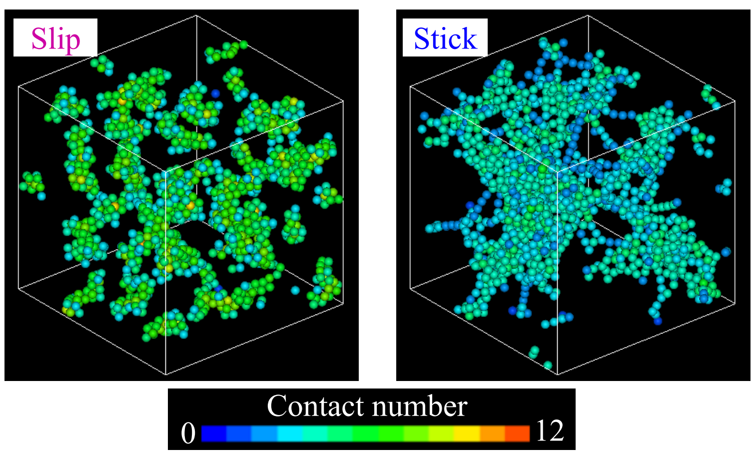

Fig. 1 Morphologies of aggregated particles without and with interparticle adhesion: slip and stick. The contact number of particles is represented by different colors.

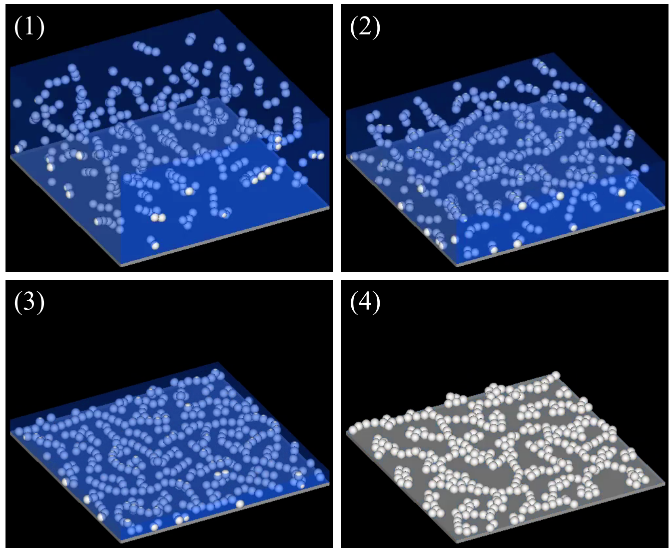

Fig. 2 Formation of a particle network during drying.

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