Numerical Simulation of Non-Equilibrium Structure Formation in Concentrated Nano-fluids

Yukio Yamaguchi, Osamu Koike, Rei Tatsumi
Department of Chemical System Engineering, The University of Tokyo.
2-11-16 Yayoi, Bunkyo-ku, Tokyo, Japan
yukiyama@sogo.t.u-tokyo.ac.jp
Presented at the 18th International Coating Science and Technology Symposium,
September 18-21, 2016, Pittsburgh, PA

Most of the problems in the manufacturing processes of functional materials are related to the non-equilibrium structure formation of concentrated colloidal solutions. There are a lot of fabrication processes shown in Figure 1 such as transporting, filtering, dispersing, kneading, coating, and drying. The particle shapes such as sphere, needle, and plate are employed in a fabrication process. The size of particles distributed from 10nm to 10 μm are usually employed. The surface of particles are adsorbed by a binder polymer or by a surfactant. [1] We have developed a numerical simulation, SNAP (Structure of NAno Particles) for several years. [2][3] Recently, the direct simulation of drying colloidal solutions on a substrate is developed using an immersed free surface model. [4]

SNAP can simulate non-equilibrium structures of concentrated colloidal solutions under non-equilibrium processes such as coating, drying, dispersing, and filtering. The functions such as conduction, transparency, and diffusivity can be estimated from the structures predicted by SNAP. The mechanism of non-equilibrium structure formation from colloidal solutions can be revealed from the simulation results by SNAP. For example, we successfully figured out the features of the shear thickening transition after the shear thinning. The shear thickening transition is elucidated as one of the non-equilibrium phase transitions due to fluid force.

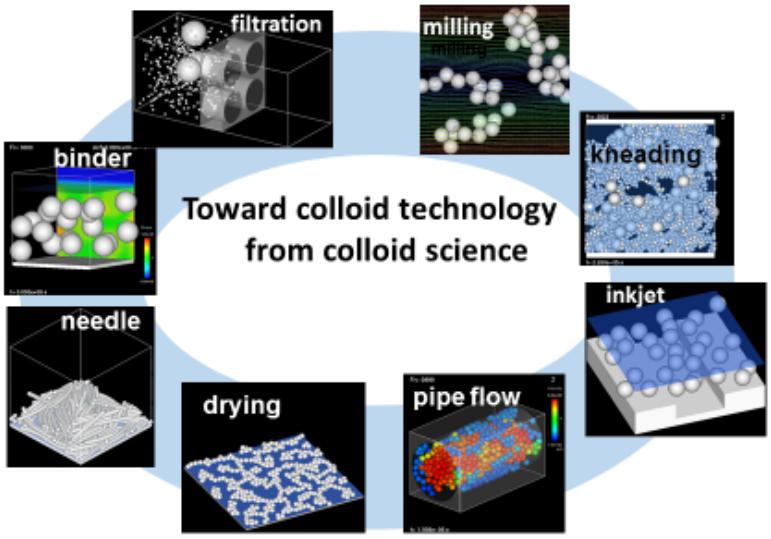

Figure 1. The applications of SNAP.

References

[1] Rei Tatsumi, Osamu Koike, and Yukio Yamaguchi, Phys. Rev. E **91**, 063301 (2015).
[2] M. Fujita, Osamu Koike, and Y. Yamaguchi, Physical Review E **77** (2), 026706 (2008).
[3] SNAP, http://nanotech.t.u-tokyo.ac.jp
[4] Masahiro Fujita, Osamu Koike, and Yukio Yamaguchi, Journal of Computational Physics 281, 421–448 (2015).