Modeling and Simulation of self oscillating gel - toward a molecular gel robot

Hiroshi Morita[1]
h.morita@aist.go.jp

Yusuke Hara[1]
y-hara@aist.go.jp

[1] Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba, Ibaraki, 305-8568, Japan

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The self-oscillating gel is one of the interesting applications of the gel with the swelling-shrinking dynamics. The self-oscillating gel is the gel which pulsates spontaneously itself using the dynamics of BZ reaction inside the gel, and it is now developing as materials for actuators or soft robots. To use self-oscillating gel as these materials, we need much precise design of functions and properties, and encounter much more difficulties. For the purpose of the precise designing of the self-oscillating gel, we make the model for self-oscillating gel, and performing these simulations.

In the dynamics of self-oscillating gel, swelling and shrinking dynamics occur repeatedly, and in these dynamics the solvents and the polymers moves inside the gel. To model the self-oscillating gel, we must treat both dynamics of solvents and polymers.

In this study, the model of self-oscillating gel based on dissipative particle dynamics (DPD) [1] method is constructed on OCTA system[2], which is the multi-scale simulation system for soft materials in the meso-scale. The swelling-shrinking dynamics was represented by changing the interaction parameter between polymer and solvent particles. In the simulations, the frequency of the changing the interaction parameter can be controlled, and with changing its frequency, the structure and the dynamics of gel can be observed. In the slower frequency case, gel can take almost equilibrium structure at each time and the change of size of gel in the swelling-shrinking cycle is much larger, however in the faster case, the movement of solvents and polymers cannot follows along the change of the interaction parameter and the delay of phase of the swelling-shrinking dynamics occurs. Noted that our model follows the previous theoretical model of gel, stress-diffusion coupling model [3], which can be applicable to the many kinds of dynamics of gel widely.

Our model is also applied to the peristaltic motion of gel. This is one of the models of worm or soft molecular robot. Our simulations indicate that our worm-like gel moves with pulsating. Our model indicates that our gel model is swimming in the solvent using the power of the BZ reaction. Detail of our simulation results and some movies will be shown in the session.

References

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