Outline of research accomplishments

In so-called “soft materials” such as liquid crystals, polymer solutions and colloidal suspensions, there exist meso-structures such as interfaces, disclination lines, entanglements of polymers and wetting layers. Since such meso-structures can be easily deformed with weak external force and relax very slowly after removal of the external force, it is easy to observe the dynamics experimentally. Moreover many soft materials exhibit the critical phenomena in phase transition under ordinary temperature and normal pressure. Thus, “soft materials” have served as one of the best fields to study phase transition dynamics as well as non-linear and non-equilibrium physics.

Some of the important problems in soft material physics are as follows:

1. “How can we describe phase transition and critical phenomena?”
2. “How do the meso-structures move in non-equilibrium environments?” and
3. “How do such motions influence macroscopic flow property (rheology) of the soft material?”

I studied these issues by constructing and analyzing hydrodynamic models that describe relevant mesoscopic degrees of freedom.

Topic 1. Self-propelled motion of a fluid droplet driven at the interface under chemical reaction

In recent years, several models of self-propelling particle have been studied in relationship with cell-motility and collective motion in a fish school or a herd of animals. It is a generic non-equilibrium bifurcation phenomenon that a particle in an isotropic environment spontaneously chooses one direction and undergoes self-propelling motion without external directional force. As a much simpler example, self-propelled motion of a droplet due to the Marangoni

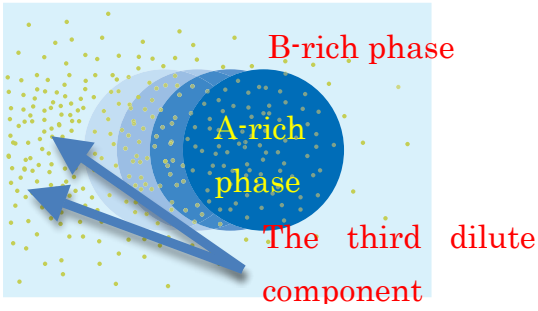

Fig. 1: A schematic figure of our model. Yellow dots represent the third component that is generated inside A-rich droplet (shown by a blue circle and undergoing self-propelled motion) and influences the interface tension of the droplet.

effect (Flow induced by gradient of interface tension) has been studied experimentally in many systems. However, even for them, there have been no hydrodynamic theories that describe bifurcation behavior of droplet velocity. We constructed a hydrodynamic model for a self-propelling fluid droplet as shown in Fig. 1. (S. Yabunaka, T. Ohta, and N. Yoshinaga, J. Chem. Phys. (2012): A copy of this paper is attached.)

We consider an A-B binary mixture and also assume the existence of a third dilute component that is generated inside the droplet and decomposed at some rate. Also we consider cases in which there is an isolated A-rich droplet. The third dilute component is assumed to increase the interface tension of the droplet. Then, if the composition of the third dilute component is not uniform on the surface of the droplet, surface force arises there and generates a flow field that transports the droplet itself. If such flow field and droplet motion reinforce the anisotropy of the third dilute component in turn, self-propelled motion can occur.

Topic 2. Dynamics of electric double layers in the presence of ion-solvent interactions (selective solvation effects)

Structure formation due to ions plays an important role in dynamics of biomaterials, such as proteins, and soft materials such as colloidal suspensions. There have been many theoretical studies on this topic without taking into account ion-solvent interactions and physical significance of ion-solvent interaction remains still elusive.

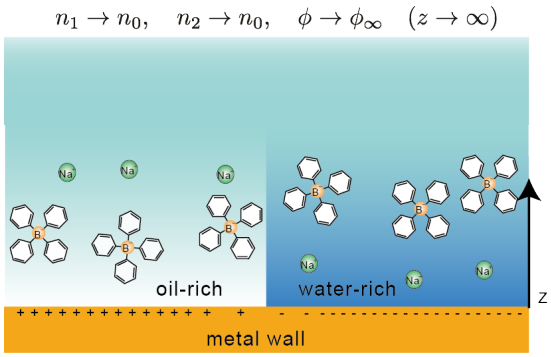

Fig. 2 Schematic representation of lateral coexistence of two one-dimensional solutions near a charged metal wall.

In liquid water, small metallic ions are surrounded by several water molecules to form a hydration shell due to the ion-dipole interaction. As a result, such ions are strongly hydrophilic. On the other hand, some ions are strongly hydrophobic. As an example, tetraphenylborate BPh4- with an 0.9nm has four phenyl rings and, due to its large size, it deforms hydrogen bonding,

leading to strong hydrophobicity.

I considered a mixture solvent (water-oil) with hydrophilic and hydrophobic ions near a charged metal wall in collaboration with Prof. Onuki (Kyoto University) (A. Onuki, S. Yabunaka, T. Araki and R. Okamoto, Current Opinion in Collioid Interface Science (2016)). Assuming that the system is uniform parallel to the wall, it reduces to a one-dimensional problem. I calculated equilibrium profiles of ion concentrations and composition.

After completing this paper, we found that the surface voltage generally behaves as a nonmonotonous function of the surface charge due to the inversion of the electric double layer near the wall. This behavior indicates thermodynamic instability of laterally uniform one-dimensional solution. The simplest possible situation is illustrated in Fig. 2. Quite recently, we actually showed that lateral pattern formation occurs due to this instability by carrying out hydrodynamic calculations in two dimensions. (S. Yabunaka and A. Onuki, accepted for publication in Physical Review Letters, 119 118001 (2017): A copy of this paper is attached.) In terms of thermodynamics, this phenomenon is characterized as a brand new surface phase transition due to selective solvation effects, which is totally different from the well-known wetting transition. Thus I believe that this is a nontrivial example of phenomena induced by fluid–structure interactions.

Other topics

Dynamics of phase transition of a critical fluid in a confined space

It is by now widely believed that everything is known about the criticality of the O(N) models either exactly or with an accuracy that is limited only by our finite computational ability. For the Wilson-Fisher fixed point, almost all the theoretical formalisms have been tested and they all yield consistent result.

However, for the multicritical fixed points, the situation is less clear. For example, a nontrivial multicritical fixed point with two unstable directions branches from the Gaussian fixed point at d=3 dimension, below which (¥phi^2)^3 term becomes relevant. The same scenario also repeats in each

critical dimension d_n=2+2/n: a nontrivial multicritical fixed point with n unstable directions branches from the Gaussian fixed point. However, in the large N limit, only the gaussian and WF fixed points have been found in generic dimension 2<d<4 so far.

In this study, we investigate the multicritical fixed point structure of the O(N) models by means of nonperturbative (also called functional) renormalization group (NPRG) and find some surprising features. In particular, we find new nonperturbative fixed points in three dimensions (d=3) as well as at N=¥infty (S. Yabunaka and B. Delamotte, Phys. Rev. Lett. 119 (19), 191602 (2017) A copy of this paper is attached.). These fixed points come together with an intricate double-valued structure when they are considered as functions of d and N. Many features found for the O(N) models are shared by the O(N)¥otimesO(2) models relevant to frustrated magnetic systems. (S. Yabunaka and B. Delamotte, in preparation)

Motion of topological defects under non-equilibrium environments

Understanding the motion of topological defects is essential for the study of pattern dynamics in non-equilibrium systems. I studied motion of topological defects under non-equilibrium environments by applying the reduction method on Ginzburg-Landau models and carrying out numerical simulations in the following cases.

1. Interface and vortex motions in the two-component Ginzburg-Landau equation (S. Yabunaka, Phys. Rev. E (2014)).

2. Interface motion in phase-separated semidilute polymer solutions (S. Yabunaka, J. Stat. Mech. (2012)).

3. Vortex motion in near-critical superfluid ^{4}He under heat flow and gravity (S. Yabunaka and A. Onuki Phys. Rev. B (2010)).