The A3 mini-Workshop on Soft matter

Beihang University, Beijing, China, Mar 23-25, 2016

Program

March 23, 2016, Afternoon

15:00-15:50   Anchang Shi (McMaster Univ.)
               Complex ordered phases of multiblock copolymers
15:50-16:20   Toshihiro Kawakatsu (Tohoku Univ.)
               Phase separation dynamics of polymer blends and blockcopolymer systems
16:20-16:40   coffee break
16:40-17:30   Kenji Yasuoka (Keio Univ.)
               Molecular Simulation of Polymer and Liquid Crystal
18:30   Diner

March 24, 2016, Morning

09:00-09:50   Jaeup Kim (UNIST)
               Self-Consistent Mean Field Theory of Polymers: Algebraic Test of Material Conservation and a Few Applications
09:50-10:20   Lei Zhang (PKU)
               Recent Developments in Computational Modeling of Nucleation in Phase Transformations
10:20-10:50   coffee break
10:50-11:40   Jinhae Park(Chungnam National University)
               A survey on Landau-de Gennes Theory of Liquid Crystals and Interface Problems
11:40-14:00   lunch

March 24, 2016, Afternoon

14:00-14:50　　Xiaoping Wang (HKUST)
　　　　　　　　Analysis of speed dependent contact angle hysteresis
14:50-15:20　　Karel Svadlenka (Kyoto Univ.)
　　　　　　　　On a penalty method for volume preserving interface motions
15:20-15:50　　coffee break
15:50-16:20　　Hisashi Naito (Nagoya Univ.)
　　　　　　　　Discrete geometric analysis and fullerene structures
16:20-16:50　　Wonju Jeon(KAIST)
　　　　　　　　Scattering Pattern of Acoustic Wave from an Anisotropic Material in Non-Uniform Mean Flow
16:50-17:20　　Kazutoshi Inoue (Tohoku Univ.)
　　　　　　　　Structure of Symmetrical Tilt Grain Boundaries
18:30　　　　　　Diner

March 25, 2016, Morning

09:00-09:50　　Xiangyang Liu (Xiamen Univ.)
　　　　　　　　Functionalization of Soft Materials Based on the Mesoscopic Materials Assembly
09:50-10:20　　Zhenli Xu (Shanghai JiaoTong Univ.)
　　　　　　　　Dielectric effects in colloidal suspensions and nanoparticle self-assembly
10:20-10:50　　coffee break
10:50-11:40　　Natsuhiko Yoshinaga (Tohoku Univ.)
　　　　　　　　Hydrodynamics and Collective Behaviors of Self-Propelled Particles and Drops in Active Suspensions
11:40-14:00　　lunch

March 25, 2016, Afternoon

14:00-14:50   Takashi Sakajo (Kyoto Univ)
Mathematical modeling and topological characterizations for 2D incompressible flows across the Reynolds number.

14:50-15:20   Yana Di (ICMSEC, CAS)
Theoretical Analysis for Meniscus Rise of a Liquid Contained between a Flexible Film and a Solid Wall

15:20-15:50   coffee break

15:50-16:20   Jaehong Pyo(Kangwon National Univ.)
A finite element dual singular function method to solve the Stokes equations including corner singularities

16:20-16:50   Xianmin Xu (ICMSEC, CAS)
A variational approach for sliding fluid on substrates

18:00   Farewell Dinner

Titles and Abstracts

Complex ordered phases of multiblock copolymers

An-Chang Shi (Department of Physics & Astronom,McMaster University)

Self-assembly of multiblock copolymers presents a great opportunity to generate tailored polymeric materials with hierarchically ordered nano-scale domains. At the same time, the phase complexity of multiblock copolymers presents a great challenge to experimental and theoretical study of their phase behavior. Theoretically the self-consistent field theory (SCFT) provides a powerful framework for the study of inhomogeneous polymeric systems. In particular, many researchers have demonstrated that SCFT can be used to describe the phase behavior of block copolymers. Our recent research focuses on the development of theoretical and simulation methods for the prediction of block copolymer phases, resulting in a generic strategy to discover complex ordered phases of block copolymers within the SCFT framework. Specifically, the strategy utilizes a combination of real-space and reciprocal-space techniques to explore possible ordered phases that could be formed by multiblock copolymer melts, resulting in an array of candidate structures. A comparison of the free energy of the candidate phases can then be used to construct phase diagrams. Our extensive calculations have demonstrated that this strategy could be used to predict the formation of complex and hierarchically ordered phases from multiblock copolymers. In particular, application of this strategy to multiblock copolymers, including linear and star ABC triblock copolymers and BACBA pentablock copolymers, has led to the discovery and understanding of a rich array of ordered phases.

Phase separation dynamics of polymer blends and blockcopolymer systems

Toshihiro Kawakatsu (Department of Physics, Tohoku University)

We develop simulaton models of phase separation dynamics of polymer/blcokcopolymer systems. Hybrid approaches between models of different length scales are efficient for such problems. We combine self-consistent field theory for inhomogeneous polymer systems with molecular dynamics, phase field theory, reptation dynamics, and so on.

Molecular Simulation of Liquid Crystal and Polymer

Kenji Yasuoka (Department of Mechanical Engineering, Keio University)

In the entangled polymeric materials, a relation between chemistry, structure and dynamics is a long-standing problem. A quantitative understanding of the relation is quite useful for the optimization of design and processing of polymeric materials. Molecular dynamics simulations for atomistic and coarse-grained model are key methods to approach it. The former can provide quantitative polymeric properties by

the explicit implementation of chemical details, and the latter have a potential for accelerating simulations by the reduction or omission of chemical information. The possibility for the linkage between two models is indicated by the established universality in the response functions of polymers. In this work, we focused on the above universality and developed a simple mapping scheme which has the great potential for the reasonable linkage between atomistic and various CG models.

Liquid crystals are a phase that may be found between those of solid and liquid. There are many different types of liquid crystal phase, depending on the molecular orientational and positional order. The molecules exhibiting liquid crystal phases have an anisotropic shape such as rod-like and disk-like structures. The macroscopic structure of a liquid crystal phase is strongly influenced by the collective behavior of these molecules. Therefore, the study at the molecular scale is very important. In this research, Monte Carlo simulations of chiral liquid crystals were performed to investigate effect of elongation on their liquid-crystal structures. To investigate molecular structures obtained by these simulations, potential energy, heat capacity, orientational order parameter, radial distribution function and orientational correlation function were calculated.

Self-Consistent Mean Field Theory of Polymers: Algebraic Test of Material Conservation and a Few Applications

Jaeup Kim (UNIST)

A method to obtain self-consistent mean field solution for polymeric systems is to solve partial differential equations for partition functions of the polymer chain. Even though the statistical mechanics of polymers itself is a perfectly accurate theory, the process of numerical solution often has problems in keeping the amount of polymer materials in the system. Recently, for the purpose of tracking material conservation in the self-consistent field theory (SCFT), our research group has developed an algebraic test which uses matrix and bra-ket notation. The test reveals that when Crank-Nicolson method is adopted, finite volume method (FVM) is the only way to conserve material perfectly in the cylindrical and spherical coordinate systems. Alternating direction implicit method combined with FVM cannot conserve material, though it is still a good candidate after considering speed and accuracy simultaneously. We also confirm that the widely used pseudospectral method in Cartesian coordinates has the ability to conserve material.

In this presentation, I will also demonstrate how one can use SCFT to analyze various experimental systems. In one example, the mixing of short random copolymers enhances the long range order of block copolymer domains. It is shown that localized disordered state at the defects greatly relieves the energy penalty for the chain diffusion and lamellar reorganization, and thus they trigger anomalously large grain growth of lamellar morphology in the block copolymer thin films.

Recent Developments in Computational Modeling of Nucleation in Phase Transformations

Lei Zhang (Beijing International Center for Mathematical Research,
          Center for Quantitative Biology, Peking University)

Nucleation is one of the most common physical phenomena in physical, chemical, biological and materials sciences. Due to the difficulties and challenges in making direct experimental observation, many computational methods have been developed to model and simulate various nucleation events. In my talk, I will provide a sampler of some newly developed numerical algorithms that are widely applicable to many nucleation and phase transformation problems. I first describe some recent progress on the design of efficient numerical methods for computing saddle points and minimum energy paths, and then illustrate their applications to the study of nucleation events associated with several different physical systems. Nucleation is a complex multiscale problem. Development of efficient numerical algorithms and modeling approaches is bringing new light to this challenging subject.

A survey on Landau-deGennes Theory of Liquid Crystals and Interface Problems

Jinhae Park(Chungnam National University)

In this talk, we shall begin with a brief introduction to the Landau-de Gennes theory of Liquid Crystals for those who are not familiar with liquid crystals. The theory can explain many physics phenomena which cannot be described by the classical Oseen-Frank theory. We plan to discuss several mathematical issues on the theory and also talk about interface problems between different phases.

Analysis of speed dependent contact angle hysteresis

Xiaoping Wang(HKUST)

We study the interface dynamics and contact angle hysteresis in a two dimensional, chemically patterned channel described by the Cahn-Hilliard equation with a relaxation boundary condition. A system for the dynamics of the contact angle and contact point is derived in the sharp interface limit. From the behaviour of the solution of the contact angle dynamic equation, we observe stick-slip motion and contact angle hysteresis. Our analysis reveals the mechanism for the asymmetric speed dependent contact angle hysteresis observed experimentally.

On a penalty method for volume preserving interface motions

Karel Svadlenka (Department of Mathematics, Kyoto University)

We propose a numerical method for computing interfacial motions with global constraints, such as volume preserving mean curvature flow, which is applicable even in the case of multiple phases. We give an outline of the related convergence analysis and show simple simulation results.

Discrete geometric analysis and fullerene structures

Hisashi Naito (Department of Mathematics, Nagoya University)

I talk about fullerene structures from viewpoints of discrete geometric analysis. In particular, I consider "negatively curved fullerens (schwarties)" by using arguments of variational problems and topological crystals.

Scattering Pattern of Acoustic Wave from an Anisotropic Material in Non-Uniform Mean Flow

Wonju Jeon(KAIST)

In this talk, we investigate the effect of fluid convection to the scattering pattern of sound wave encountering a material with anisotropic physical properties. A moving medium wave equation adequate to the study of wave refraction due to non-uniform mean flow is introduced and the effect of non-uniformity within flow is examined aiming at the design of a future silent aircraft and a new defense technology.

Structure of Symmetrical Tilt Grain Boundaries

K. Inoue[1*], M. Saito[2], M. Kotani[1] and Y. Ikuhara[1,2]

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Intensive studies have been carried out since several decades ago to unravel complicated structures of grain boundaries (GBs) which can be formulated as an arrangement of 1-dimensional defects. After the successful formulation of the coincidence-site-lattice theory, GBs have been classified by the coincidence index Σ and GBs of high index are often found to show an arrangement of energetically stable sub-structures with low index, which can be well described by a dislocation-based model. On the other hand, GBs energy, as a function of the misorientation, can be well predicted by the disclination-based model.

It was found that the periodicity of SUs in a symmetrical tilt grain boundaries (STGBs) are closely related to the distribution of irreducible rational numbers [1]. As a generalization, the structures of STGBs for any misorientation can be well approximated in a given precision by the Farey sequence [2].

[1] K. Inoue, M. Saito, Z.W. Wang, M. Kotani and Y. Ikuhara, Mater. Trans., 56(3), 281-287, (2015).
[2] K. Inoue, M. Saito, Z.W. Wang, M. Kotani and Y. Ikuhara, Mater. Trans., 56(12), 1945-1952, (2015).

Functionalization of Soft Materials Based on the Mesoscopic Materials Assembly

Xiangyang Liu(Research Institute for Biomimetics and Soft Matter, Xiamen University, Department of Physics, Faculty of Science, National University of Singapore)

For many functional materials of complex structures, the functionality that is critical to macroscopic behavior begins to manifest itself at the mesoscale. In order to control the macroscopic properties, the knowledge on the structural characteristics in relationship to the properties of mesoscopic materials becomes then very crucial. As crystal networks are one of key mesoscopic structures encountered frequently, I will in this presentation provide a systematic and comprehensive survey on the structural characteristics of crystal networks in correlation with the macroscopic properties/performance, and the formation mechanisms and engineering strategy of mesoscopic materials. In this regard, the hierarchy of crystal network structures: crystal network and domain network, turns out to be the basic features of crystal networks. It was first decribed by the four factors, the topology, correlation length, symmetry/ordering, and strength of association of crystal networks, which determine the macroscopic behavior of mesoscopic materials. According to the principle of materials engineering triangle, the formation of crystal networks should be understood. In this regard, the basic mechanisms of crystal nucleation and growth were first reviewed. These are further extended to the formation of multi levels of crystal networks. Three major pathways of crystal network construction are discussed in detail. Consequently, the engineering of mesoscopic materials can be implemented by tuning the four factors of crystal networks in terms of additives, sonication, seeding, thermodynamic driving force etc. To demonstrate the outlined principles, the correlation between the mesoscopic structure and the performance of biominerals, the engineering of molecular gels were overviewed. Furthermore, the large breaking stress and strain of spider silk were explained and predicted within the framework of hierarchical breaking mechanism, ordering, correlation length, the hierarchical structure and strength of nano-fibrils. Evidently, the comprehensive knowledge on crystal networks will guide the research of mesoscopic materials in the long term.

Dielectric effects in colloidal suspensions and nanoparticle self-assembly

Zhenli Xu(Shanghai Jiaotong University)

Dielectric-interface effects are many-body effects and play important role in many soft matter, energy device, and biological systems at the nano/micro scale. We have developed a fast algorithm for electrostatic interaction in the presence of many dielectric spheres and ions, which can be densely (close to touching) packed. The algorithm is a hybrid method of the method of moments and image charges. By using the FMM acceleration, the algorithm is shown promising for particle simulations of colloids and nanoparticles in ionic environments. We reported the results on colloidal suspensions and nanoparticle self-assembly by using the molecular dynamics simulations to show the role of dielectric effects in these physical systems and also show the attractive performance of the new simulation method.

Hydrodynamics and Collective Behaviors of Self-Propelled Particles and Drops in Active Suspensions

Natsuhiko Yoshinaga (WPI-AIMR, Tohoku University)

Spontaneous motion has attracted lots of attention in the last decades in fluid dynamics for its potential application to biological problems such as cell motility. Recently, several model experiments showing spontaneous motion driven by chemical reactions have been proposed and revealed the underlying mechanism of the motion. Accordingly, several simple theoretical models have been extensively studied such as active Brownian particles, squirmers, self-thermophoretic swimmers and so on. We theoretically derive a set of nonlinear equations showing a transition between stationary and motile states driven away from an equilibrium state due to chemical reactions. A particular focus is on how hydrodynamic flow destabilizes an isotropic distribution of a concentration field. It is of interest that due to self-propulsive motion and flow around the droplet, a spherical shape becomes unstable and it elongates perpendicular to the direction of motion.

The assemblage of such self-propelled particles may show collective behaviors and dynamical patterns. The particular focus is on how hydrodynamic interactions and the interaction mediated by a concentration field give rise to collective behaviors such as motility-induced phase separation, global polar state, and clustering. Even for the simpler models of self-propelled particles and drops, our understandings of their interactions are still primitive. I shall argue these issues based on our recent results of theoretical calculations.

Mathematical modeling and topological characterizations for 2D incompressible flows across the Reynolds number.

Takashi Sakajo (Department of Mathematics, Kyoto University)

In material sciences and life sciences, there arise many research topics related to fluid phenomena such as metal alloys and nano-devices, bird/insects flights and movements of bacteria/sperms. It is sometimes useful to consult simple mathematical models to understand these phenomena theoretically, by which one can extract qualitative mathematical structures that lie behind them. The present talk consists of two parts. In the first part, I will provide a brief review of recent developments on mathematical modeling techniques for 2D flows with the theory of complex analysis. Here, we assume that the fluid is incompressible and it is confined in domains of two dimensions, but we can flexibly deal with two extreme situations when the viscosity is negligibly small and when it is very strong. In other words, it enables us to construct mathematical flow models across the Reynolds numbers: from flows of birds/insects flights to flows of micro-swimmers and nano-devices. Mathematically, 2D incompressible flows, regardless of their viscosity, are described by holomorphic functions, to which we can make the best use of the beautiful theory of complex functions. In addition to the theoretical advantage, recent developments of numerical analysis allow us to compute and visualize these complex functions fast and accurately, which opens a new branch of research area called Applied and Computational Complex Analysis (ACCA). In the second part, based on the fact that each 2D incompressible flow defines a Hamiltonian vector field with the stream-function being its Hamiltonian,

I will provide a mathematical theory of topological pattern characterizations for 2D incompressible flows that has recently been developed in our research project. It enables us to identify topological flow patterns, i.e. streamline patterns, with simple symbolic expressions called maximal words and regular expressions. The symbolic descriptions bring us new qualitative information on the correspondence between flow patterns and their functions/evolutions, that are applicable to many flow phenomena appearing in material and life sciences.

Theoretical Analysis for Meniscus Rise of a Liquid Contained between a Flexible Film and a Solid Wall

Yana Di (ICMSEC, CAS)

We study the dynamics of meniscus rise of a liquid contained in a narrow gap between a flexible film and a solid wall. We show that the meniscus rises indefinitely expelling liquid from the gap region, and that the height of the rising front   increases with time as , while the gap distance $e(t)$ decreases as .   These results are consistent with the experiments of Cambau.

A finite element dual singular function method to solve the Stokes equations including corner singularities

Jaehong Pyo(Kangwon National Univ.)

Abstract. The finite element dual singular function method [FE-DSFM] has been constructed and analyzed accuracy by Z. Cai and S. Kim to solve the Laplace equation on a polygonal domain with one reentrant corner. In this paper, we impose FE-DSFM to solve the Stokes equations via the mixed finite element method. To do this, we compute the singular and the dual singular functions analytically at a non-convex corner. We prove well-posedness by using the contraction mapping theorem and then estimate errors of the algorithm. We obtain optimal accuracy O(h) for velocity in $H^1(\Omega)$ and pressure in $L^2(\Omega)$, but we are able to prove only O($h^{1+\lambda}$) error bounds for velocity in $L^2(\Omega)$ and stress intensity factor, where λ is the eigenvalue. However, we get optimal accuracy results in numerical experiments.

A variational approach for sliding fluid on substrates.

Xianmin Xu(ICMSEC,CAS)

A variational method is introduced to calculate the evolution of liquid film and liquid droplet moving on a solid substrate. An explicit time evolution equation is obtained for the contact angle of a liquid film that starts to move on a horizontal substrate. The equation predicts the dynamical transition at the receding side, and the ridge formation at the advancing side. The same method is applied for the evolution of a droplet that starts to move on an inclined solid surface, and again the characteristic shape change of the droplet is obtained. This demonstrates the potentiality of the present method to wider classes of problems of sliding liquids which involve contact line pinning, surface tension gradients and evaporation etc.