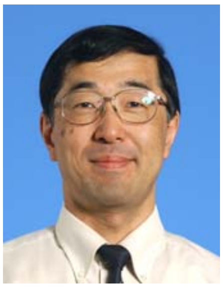
【Grant-in-Aid for Scientific Research(S)】
Science and Engineering (Mathematical and physical sciences)



Title of Project : Hierarchical Self-Organization and Dynamics of Liquids

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Research Area : Biophysics/Chemical physics
Keyword : Chemical Physics, Soft Matter Physics

【Purpose and Background of the Research】

A liquid state is one of the most fundamental and useful states of matter and its deeper understanding will have large impact on various fields of science, physics, chemistry, materials science, and bioscience. Despite its importance, however, its physical understanding lags far behind other fundamental states, gas and crystal states.

In this project, we study the following unsolved fundamental problems in liquid science:(1) Thermodynamic and kinetic anomaly of water and water-like liquids. (2) Mechanism of liquid-liquid transition in a single-component liquid. (3) Mechanism of liquid-glass transition. (4) Relationship between a hierarchical structure of liquid and its crystallization. (5) Nonlinear flow behavior of glassy and granular matter and the fracture mechanism.

So far simple liquids have been studied from a microscopic viewpoint, focusing on the single-particle-level structure and dynamics. This is natural if the particle size is the only lengthscale. We believe, however, that many unsolved problems in liquid science, which were mentioned above, arise from a spatio-temporal hierarchical structure of liquid, which extends beyond a particle size (see Fig. 1).

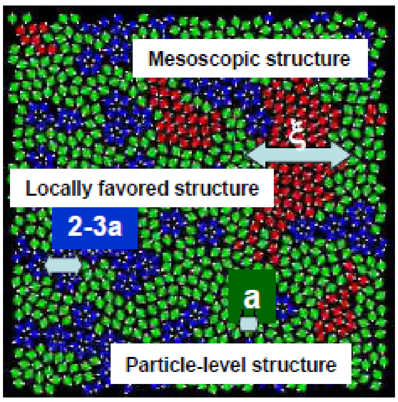

Fig. 1 Hierarchical structure of a supercooled liquid

【Research Methods】

We are planning to study the above topics (1)-(5), focusing on (i) the tendency of liquid molecules to form locally favored structures and crystal-like order and (ii) the competition between these two types of orderings. We plan to combine experimental approaches (real-space and wavenumber-space structural and dynamical characterization and spectroscopic & thermal measurements) with numerical (Brownian dynamics, molecular dynamics, and fluid particle dynamics methods) and theoretical approaches.

【Expected Research Achievements and Scientific Significance】

Liquid plays crucial roles in bio- and chemical reactions and a number of industrial processes. If we can control various physical (density, refractive index, viscosity, …) and chemical (reactivity, miscibility, …) properties of a liquid by transforming a liquid to another liquid by external fields (temperature, pressure, flow, light, …) using liquid-liquid transition, the impact would be dramatic. Furthermore, if we can reveal instability mechanisms of liquid, glassy matter, and granular matter under shear deformation, we may predict the onset of instability (cavitation of liquid and fracture of amorphous materials) and slipping of flow in a confined liquid. This may also contribute to our basic understanding of the rule governing the state selection under nonequilibrium situations.

【Publications Relevant to the Project】

- H. Shintani and H. Tanaka, Frustration on the way to crystallization in glass, Nature Phys. 2, 200-206 (2006).
- R. Kurita and H. Tanaka, Critical-like phenomena associated with liquid-liquid transition in a molecular liquid, Science 306, 845-848 (2004).
- C. P. Royall, S. R. Williams, T. Ohtsuka and H. Tanaka, Direct observation of a local structural mechanism for dynamic arrest, Nature Mater. 7, 556-561 (2008).

【Term of Project】 FY2009-2013

【Budget Allocation】 151,800 Thousand Yen

【Homepage Address and Other Contact Information】

http:// tanakalab.iis.u-tokyo.ac.jp/