# Exhaustive Structure Search in Supercooled Liquids

Masakazu Matsumoto* and Motoshi Kamiya
*Department of Chemistry, Nagoya University*

Although the dynamical heterogeneity is recognized as a common phenomenon in supercooled liquids leading to glass transition, its structural origin is not quite understood.[1] It is partly because we don't have a universal method to describe the local order and structural heterogeneity in the liquids.

Glass transition is observed under the condition where crystallization is inhibited. In this sense, crystallization and glass transition are strongly related. It is important, therefore, to explain what kind of local structure prevents the system from forming crystalline nucleus and keeps (meta)stable to be glassy. There are many candidates of locally preferred structures. Some structures are known as a part of stable crystal forms, while there are many other possibilities, e.g. (unidentified) metastable crystals, quasicrystals, amorphous states, etc. Thus the method to find the locally preferred structures without prior knowledges is wanted.

We introduce an exhaustive search of locally stable structures with the use of graph matching and pattern classification to the supercooled liquids. As an example, structure and topology of network-forming materials, supercooled water and liquid silicon, is elucidated.[2] Their structure is found to be an aggregate of polyhedral network motifs without frustration. The mechanism of self organization leading to the liquid-liquid coexistence of water and silicon is explained in terms of matching and packing of these polyhedral network motifs.

This concept of exhaustive search without prior knowledges is also applicable to supercooled simple liquids. It is found that the molecular mobility is related with local order and that the dynamical heterogeneity is governed by the structural heterogeneity.

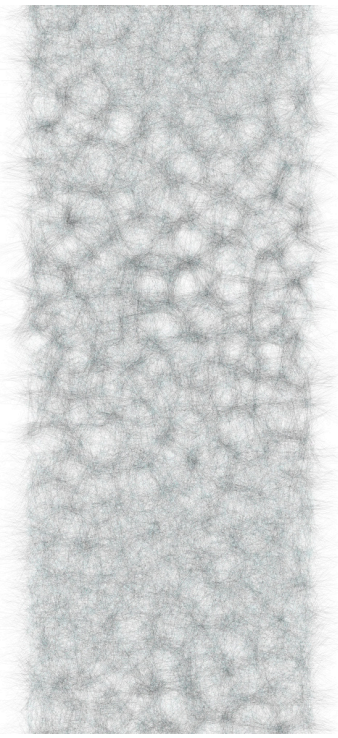

FIG.1: Hydrogen bond network of supercooled water under pressure is superposed over 400 ps. Stable and ordered domain is apparent.

* Corresponding author: matto@nagoya-u.jp

[1] R. Yamamoto and A. Onuki, Phys. Rev. E 58, 3515 (1998).
[2] M. Matsumoto: A. Baba, and I. Ohmine, J. Chem. Phys. 127, 134504 (2007).