Real-space analyses of liquid dynamics using high energy-resolution inelastic X-ray scattering

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The conventional approach to the study of the liquid dynamics is to measure the dynamic structure factor, $S(Q, \omega)$, where Q and $E=\hbar\omega$ are the momentum transfer and energy transfer, by inelastic X-ray or neutron scattering and to fit models in Q-ω space to interpret the data. For the systems which lack periodicity in their atomic structures, analyses in reciprocal space are sometimes powerless in describing their structure and dynamics and the real-space analyses can provide their local information as has been demonstrated in the structural analyses using pair-distribution function. Recent progress in inelastic X-ray scattering makes it possible to obtain inelastic scattering spectra over a wide range of Q and E with a high Q- and E-resolution within a reasonable amount of time. The wide Q- and E-ranges make it possible to calculate the self-part and the distinct-part of the Van Hove function–spatial and temporal correlation function [1]–via Fourier transform of $S(Q, \omega)$ over ω and Q [2]. With this approach, we have studied spatial and temporal correlations of molecular motion in liquids [2–4]. In this presentation, our recent efforts in understanding the real-space local motion in liquids using the Van Hove function will be presented.

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