Microscopic Structure and Dynamics in Ionic Glass $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$: Quasi-Elastic Gamma-Ray Scattering and X-Ray Diffraction Studies

Makina SAITO[1], Yohei ONODERA[1], Ryo MASUDA[1], Yoshitaka YODA[2], and Makoto SETO[1]

[1]*Institute for Integrated Radiation and Nuclear Science, Kyoto University, Kumatori, Osaka, Japan*

[2]*Research and Utilization Division, Japan Synchrotron Radiation Research Institute, Sayo, Hyogo, Japan*

When liquids are cooled toward the glass transition, viscosity or the time scale of the microscopic diffusional process (called as the α process) increases rapidly without apparent structural change. Therefore, the glass transition phenomenon is characterized by the microscopic dynamics. In glass state, the α process almost freezes; however the local jumping process called as the Johari-Goldstein (JG) β process still occurs in the time scale of *e.g.,* micro-second and thought to be a primitive process for the ion conducting in the ionic conductors.[1] However, the microscopic dynamical picture of the JG-β process is hardly known owing limitation of both experiment and simulation.

We developed quasi-elastic gamma-ray scattering (QEGS) spectroscopy, which allows for the measurement of the microscopic ionic dynamics directly via obtaining the intermediate scattering function $S(q,t)$ in the time scale between nano-second and micro-second, where q is the momentum transfer.[2] For the first trial of characterization of the JG-β process, we studied a typical glass forming system $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$ (CKN) using QEGS at BL09XU of SPring-8 and $S(q,t)$ is obtained at various q points. In addition, we performed X-ray diffraction experiment on CKN at BL04B2 of SPring-8 and reverse Monte Carlo (RMC) modelling for the obtained static structure factor. The partial static structure factor estimated by the glass structure modeled by RMC has information of the contribution weight of each atom for scattering at q. By analyzing $S(q,t)$ based on the structural information, we could evaluate the time scale of all ionic motion (translational and rotational motion). Consequently, we found both rotational and translational motions contribute to the JG-β process in CKN. We developed the way to quantitatively characterize a microscopic ionic/atomic motion in glasses.

REFERENCES

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