Atomic and electronic structures of functional disordered materials revealed bycomprehensive integration of theoretical, experimental, computational and data-centric sciences

Shinji Kohara（National Institute for Materials Science, Principal Researcher)

（FY2017-2020）

Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

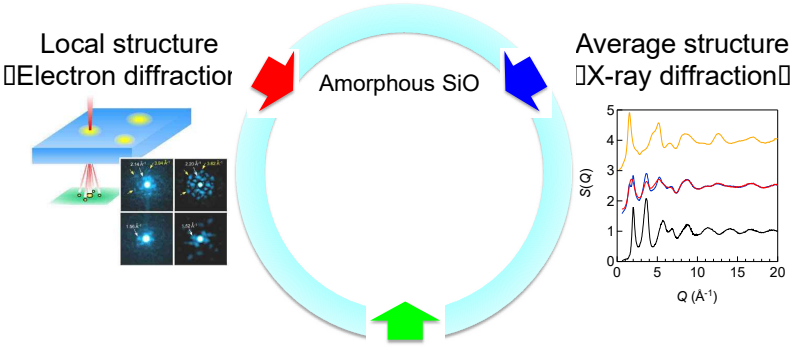
Brief overview

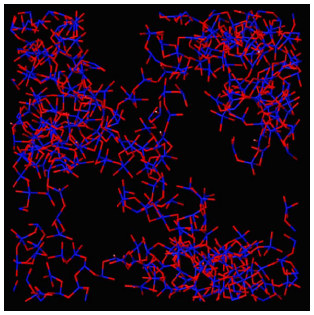
The structure of glassy, liquid, and amorphous materials is still not well understood, due to the lack of structural information hidden in pairwise correlations. In this research, a comprehensive integration of theoretical, experimental, computational and data-centric sciences is realized, in order to uncover the atomic structure of functional disordered materials, under ambient to extreme conditions, e.g., high temperature and high pressure. Moreover, attempts will be made to extract the relationship between structure and function with special focus on network, ring statistics, cavity, and homology.

Achievements

We have succeeded in modelling the disproportionation of an amorphous battery electrode (silicon monoxide) by a combination of measurements and simulations. We have revealed the network structure in binary phosphate glasses, which are mother materials for low-melting point glasses, by data-driven structure modelling based on X-ray/neutron diffraction and NMR spectroscopic data. The formation of a Zn-O polyhedral network was discovered, which can explain the anomalous behavior of the thermal expansion coefficient in these glasses.

Disproportionation of amorphous silicon monoxide (SiO)





Formation of the Zn-O polyhedral network discovered in the ZnO-P_2O_5 glass, that can explain the anomalous behavior of the thermal expansion coefficient

Red：oxygen

Blue：zinc

Reference/Link

A. Hirata, S. Kohara, T. Asada, M. Arao, C. Yogi, H. Imai, Y. Tan, T. Fujita and M. W. Chen, Nat. Commun. 7, 2016, 11591.
https://www.natureasia.com/ja-jp/ncomms/abstracts/76416
Y. Onodera, S. Kohara, H. Masai, A. Koreeda, S. Okamura and T. Ohkubo, Nat. Commun. 8, 2017, 15449.