Modification of Phosphate Network in binary zinc phosphate glass

Yohei ONODERA[1,2], Shinji KOHARA[3,2,4], Hirokazu MASAI[5], Akitoshi KOREEDA[6], and Takahiro OHKUBO[7]

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

[2]*Center for Materials Research by Information Integration, National Institute for Materials Science NIMS), Ibaraki, Japan.*

[3] *Light/Quantum Beam Field, Research Center for Advanced Measurement and Characterization, NIMS, Sayo, Hyogo, Japan*

[4] *PRESTO, Japan Science and Technology Agency, Tokyo, Japan.*

[5] *Inorganic Functional Materials Research Institute, National Institute of Advanced Industrial Science and Technology, Ikeda, Osaka, Japan*

[6] *Department of Physical Sciences, Ritsumeikan University, Kusatsu, Shiga, Japan*

[7] *Graduate School & Faculty of Engineering, Chiba University, Chiba, Japan*

Zinc phosphate glass has significant potential for practical applications, owning to its unique physical and structural properties. Therefore, understanding the network structure of a zinc phosphate glass is one of the most important unresolved issues in glass science. In the present study, atomic structure of zinc phosphate glass ($60ZnO\text{-}40P_2O_5$ and $70ZnO\text{-}30P_2O_5$ glass) was revealed by reverse Monte Carlo modeling[1] using a combination of neutron diffraction[2], X-ray diffraction and Zn K-edge extended X-ray absorption fine structure (EXAFS) data with several chemical coordination constraints around phosphorus atoms based on ^{31}P NMR data. The network structure is found to be largely taken by PO_4 tetrahedra in $60ZnO\text{-}40P_2O_5$ glass while the connectivity of Zn-O polyhedra becomes dominant in $70ZnO\text{-}30P_2O_5$ glass[3]. This behaviour suggests that the thermal expansion coefficient is sensitive to the difference in glass structure induced by the addition of 10 mol% ZnO.

REFERENCES

[1] O. Gereben, P. Jóvári, L. Temleitner, and L. Pusztai, *J. Optelectron. Adv. Matter.*, **9**, 3021 (2007).

[2] K. Suzuya, K. Itoh, A. Kajinami, and C. K. Loong, *J. Non-Cryst. Solids*, **345**, 80 (2004).

[3] Y. Onodera, S. Kohara, H. Masai, A. Koreeda, S Okamura, and T. Ohkubo, *Nat. Commun.*, **8**, 15449 (2017).