2C/2009G605

O 2p partial density of states and local structures in oxide glasses

Shinya HOSOKAWA*[1], Hitoshi SATO[2], Kojiro MIMURA[3], Naohisa HAPPO[4], Shinji KOHARA[5]
[1]Hiroshima Institute of Technology, Hiroshima 731-5193, Japan
[4]Hiroshima University, Higashi-Hiroshima 739-0046, Japan
[3]Osaka Pref. University, Sakai, 599-8531 Japan
[4]Hiroshima City University, Hiroshima 731-3194, Japan
[5]SPring-8/JASRI, Hyogo 679-5198, Japan

Introduction

Oxide glasses have been widely used for human life for more than three thousands years, which are a group of non-crystalline materials of chemically stable. One of the typical oxide glasses is glassy silica (g-SiO_2), in which SiO_4 tetrahedra are connected with each other by corner-sharing of O atoms, and form continuous networks (network former) similar to the crystal quartz. From previous structural studies [1], the Si-O-Si bond angle is about 150°, almost rectilinear. By mixing with another oxides as network modifiers, properties of oxide glasses can easily be controlled. For example, by adding B_2O_3, the glass becomes mechanically and chemically strong and called 'Pylex' glass. The structure of glassy B_2O_3 is based on B_3O_3 hexagonal ring, where the B-O-B bond angle is 120° [2], much smaller than that in g-SiO_2. Thus, the bond angles around the O atoms may be highly modified in Pylex glass.

In this paper, we report results of O 2p partial valence-band electronic density of states (DOS) of silica and Pyrex glasses obtained by O 1s soft x-ray emission spectroscopy (XES), which is very sensitive for the local structure around the O atoms, in particular for bond angles around the O atoms.

Experimental procedure

The XES measurements were performed at BL2C of PF-KEK at room temperature on SiO_2 and Pylex glasses, as well as SiO_2 crystal (quartz), which are commercially available. In the experiment, O K core absorption was carefully measured firstly by total emission yield method to obtain information on the O 2p partial conduction-band DOS. Then, O 1s XES spectra were measured at various incident photon energies from 530.3 to 560 eV.

Results and discussion

The XES spectra of crystal and glassy SiO_2 are very similar to ach other, indicating that the local structures around the O atoms remain mostly unchanged by amorphization. The XES spectra are depicted in Fig. 1 for SiO_2 (red) and Pylex (blue) glasses at various incident soft x-ray energies. As is clearly seen in the figure, the XES spectra of Pylex glass are very different from those of g-SiO_2, in particular at the low incident photon energies. This finding suggests that the local structures around the O atoms in Pylex glass is highly modified from those in the SiO_2 network former as was expected. Theoretical analyses of these results are now in progress.

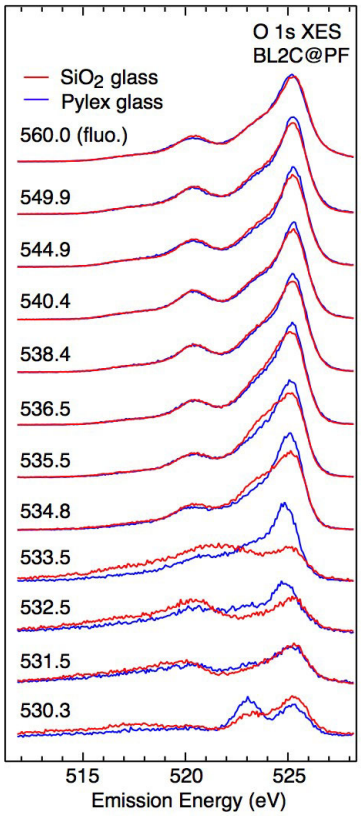

Fig. 1 O1s soft x-ray emission spectra of SiO_2 (red) and Pylex (blue) glasses.

References

[1] For example, S. Kohara and K. Suzuya, Phys. Chem. Glasses 43C, 51 (2002).
[2] F. L. Galeener, G. Lucovsky, and J. C. Mikkelsen, Jr., Phys. Rev. B 22, 3983 (1980).

* hosokawa@cc.it-hiroshima.ac.jp