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

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Introduction
Oxide glasses have been widely used for human life for more than three thousand years, which are a group of non-crystalline materials of chemically stable. One of the typical oxide glasses is glassy silica (g-SiO2), in which SiO4 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 B2O3, the glass becomes mechanically and chemically strong and called ‘Pylex’ glass. The structure of glassy B2O3 is based on B3O3 hexagonal ring, where the B-O-B bond angle is 120° [2], much smaller than that in g-SiO2. 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 SiO2 and Pylex glasses, as well as SiO2 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 SiO2 are very similar to each other, indicating that the local structures around the O atoms remain mostly unchanged by amorphization. The XES spectra are depicted in Fig. 1 for SiO2 (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-SiO2, 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 SiO2 network former as was expected. Theoretical analyses of these results are now in progress.

Fig. 1 O1s soft x-ray emission spectra of SiO2 (red) and Pylex (blue) glasses.

References
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