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

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1 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 silica (SiO_2), in which SiO_4 tetrahedra are connected with each other by corner sharing of O atoms, and form continuous networks similar to the crystal quartz. From previous structural studies [1], the Si-O-Si bond angle is about 150°, almost rectilinear. On the other hand, the structure of another typical oxide glass, B_2O_3, is based on the B_3O_3 hexagonal rings (boroxol ring), where the B-O-B bond angle is about 120° [1, 2], much smaller the that in SiO_2 glass.

It is no doubt that the bond angles around the O atoms in the oxide glasses strongly affect the electronic structures. However, the experimental investigations, such as by photoemission spectroscopy, are very difficult because these glasses are highly insulating. Soft x-ray emission spectroscopy (SXES) can provide information on valence-band density of states (DOS) of such insulating materials. However, some SXES experiments of these oxide glasses were limited to be carried out for the kation (Si [3] or B [4]) partial DOSs so far. In this paper, we report results of O 2p partial valence-band DOS of SiO_2 and B_2O_3 glasses obtained by O 1s SXES.

2 Experiment

The SXES measurements were performed at BL2C of PF-KEK at room temperature on SiO_2 and B_2O_3 glasses. In the experiments, core absorption spectra were carefully measured firstly by total emission yield method around the O *K* absorption edge of about 537 eV in order to obtain information on the O 2p partial conduction-band DOS. After then, O 1s SXES spectra were measured at various incident photon energies from about 530 to 560 eV.

3 Results and Discussion

The SXES spectra of glassy SiO_2 and B_2O_3 are shown by dashed and solid curves, respectively, at $h\nu$ = 550 eV. The intensities are reduced with respect to the peak intensities at about $h\nu$ = 525 eV. As clearly seen in the figure, the SXES spectrum of B_2O_3 glass are very different from that of SiO_2 glass. In particular, (1) the first peak emission energy is shifted towards the higher energy by about 1 eV, and (2) the sub-band structures in the lower emission energy region are much simpler. Theoretical analyses of these experimental results using an *ab initio* molecular dynamics simulation are now in progress.

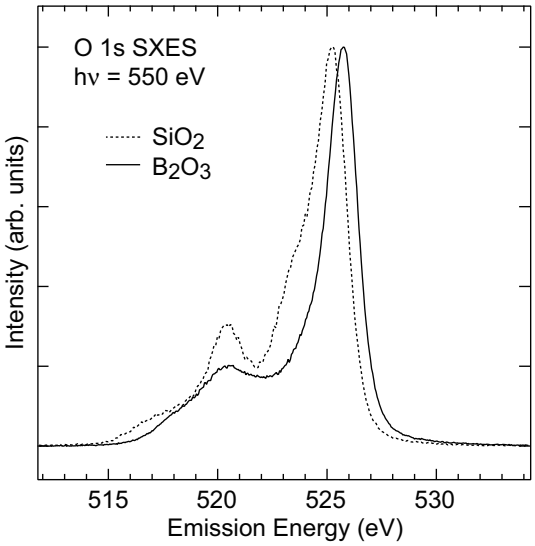

Fig. 1: O 1s soft x-ray emission spectra of SiO_2 (dashed curve) and B_2O_3 (solid curve) glasses at $h\nu$ = 550 eV.

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