Resonant photoelectron spectroscopic study of MoS$_2$ at the sulfur L-edge

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Introduction
Molybdenum disulfide (MoS$_2$) with a layered structure has long been of great interest due to the strong anisotropic character and the practical importance as a catalyst component or lubricant. In the present study, we measured the S L-edge x-ray absorption near edge structure (XANES) spectrum and resonant photoelectron spectra of MoS$_2$ to elucidate the electronic structure of MoS$_2$.

Experimental
All the measurements were performed at the beam line 13C. The S L-edge XANES spectrum was measured by the total electron yield method by monitoring the intensities of secondary electrons at normal incidence. Photoelectron spectra were obtained at photon energies of 150–191 eV and data were accumulated with a pass energy of 11.75 eV.

Results and Discussion
Figure 1 shows the S L-edge XANES spectrum of MoS$_2$ single crystal. Pre-edge features are observed at 162–166.5 eV. These features are assigned to the electron transitions from S2p$_{1/2}$ and S2p$_{3/2}$ to S4s-Mo4d antibonding orbitals, whereas the features over 167 eV correspond to the transitions above the vacuum level.

The valence band spectra of MoS$_2$ shown in Fig. 2 were measured at the photon energies of 150-191 eV. The small and broad peak near 15 eV is assigned to S3s, whereas the peaks at 5-10 eV are dominantly assigned to the S3p emissions.

With the photon energy of 166.6 eV, a small shoulder peak is observed at the higher energy side of S3s. This peak shifts to the higher binding energy side and becomes more intense with increasing the photon energy. Thus, this peak is assigned to a normal Auger decay peak of S(L$_{2,3}$VV).

With the photon energies of 163-164.9 eV corresponding to the pre-edge region, an eminent enhancement is observed in the binding energy of 9-15 eV. The peak position of this broad peak is independent of the photon energy. This indicates that the emitted electron from S2p remains at an excited state and behaves as an S(L$_{2,3}$VV) spectator in the decay process.

This process can be described simply in an atomic picture as follows.

(1) Excitation
S(2p)$^6$...S(3p)$^6$Mo(4d)$^2$ $\rightarrow$ S(2p)$^5$...S(3p)$^6$Mo(4d)$^3$

(2) Autoionization
S(2p)$^5$...S(3p)$^6$Mo(4d)$^3$ $\rightarrow$ S(2p)$^6$...S(3p)$^1$Mo(4d)$^3$ + e$^-$

Detailed analysis is now being performed to obtain more precise information on the electronic structure.

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Figure 1 S L-edge XANES spectrum of MoS$_2$ recorded at normal X-ray incidence

Figure 2 Valence band spectra obtained at S L-edge. The photon energies of each spectra are listed on the figure.