Chemical State Analysis of Si during Hydrogen Generation

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The most common industrial method of hydrogen production also produces carbon dioxide. Therefore, we focused on hydrogen production by the reaction of Si and H_2O, which does not emit greenhouse gases. In a previous study [1-3], it was found that in hydrogenated Si, the reaction with water causes a decrease in the zero-valent Si and an increase in the oxide component of Si. In the increase of the oxide component, $SiO(OH)_2$, which is different from SiO_2, is formed. However, in the previous study [1-3], the Si *K*-edge XAFS measurements were performed after the sample was once exposed to air and dried naturally after hydrogen production. In this study, a liquid cell was prepared to investigate the chemical state of Si in solution with hydrogen generation.

The XAFS measurements were carried out at BL-13 of SR Center in Ritsumeikan University. By using a liquid cell (Fig. 1), XAFS spectra of solution were obtained in the partial fluorescence yield method. As shown in Fig. 2, K *K*-edge XAFS spectrum of KCl aq. is quite different from that of KCl powder due to the different chemical environment. For the Si *K*-edge measurements, incident energies were changed by InSb(111) double crystal monochromator.

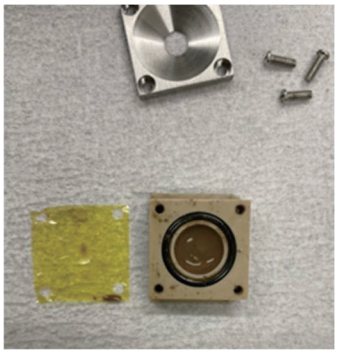

Fig. 1 Photograph of a liquid cell.

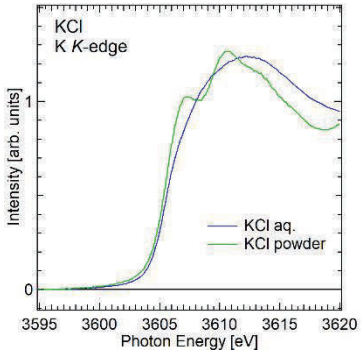

Fig. 2 K *K*-edge XAFS spectra of KCl aq. and KCl powder.

The Si *K*-edge XAFS spectra are shown in Fig. 3. For the Si powder without water, the Si^0 component is observed around 1840 eV. For the Si powder in water, the Si^{4+} component around 1847 eV appears. Note that the intensity of Si^{4+} in the Si powder after the addition of water in the previous study [1-3] was stronger than that of Si^{4+} in the liquid cell even after 3 days. In the present experimental condition, the hydrogen generation reaction was not as strong as in the previous study [1-3].

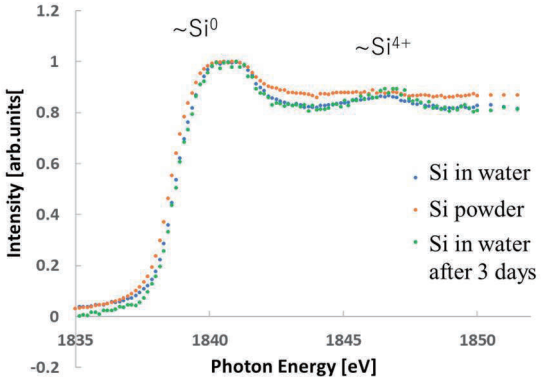

Fig. 3 Si *K*-edge XAFS spectra of Si powder with and without water.

References

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[3] Shugo Nishimura, Shiho Fujimura, Kei Mitsuhara, Masaru Takizawa, and Eiji Yamasue, *MEMOIRS OF THE SR CENTER RITSUMEIKAN UNIVERSITY*, *2020*, **22**, 49.