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Chemical State Analysis of Si in NaOH Aqueous Solutions

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The most prevalent industrial method for hydrogen production also generates carbon dioxide. Consequently, our focus shifted to hydrogen production through the reaction of silicon (Si) with water (H_2O), a process that does not emit greenhouse gases. In a prior investigation, it was observed that hydrogenated Si undergoes a reduction in zero-valent Si and an increase in the oxide component of Si upon reaction with water [1-3]. Specifically, the formation of $SiO(OH)_2$, distinct from SiO_2, occurs during this increase in the oxide component. However, in the previous study, Si *K*-edge X-ray Absorption Fine Structure (XAFS) measurements were conducted after the sample had been exposed to air and naturally dried following hydrogen production. In our current study, we employed a solution cell to explore the chemical state of Si in solution during hydrogen generation.

The XAFS measurements were carried out at BL-13 of SR Center in Ritsumeikan University. A liquid cell was employed to obtain XAFS spectra from the solution using the partial fluorescence yield method. Additionally, for Si *K*-edge measurements, the incident energies were modulated using an InSb(111) double crystal monochromator.

Figure 1 illustrates the XAFS spectra obtained from solution cells containing NaOH aqueous solutions with concentrations of 1 wt% along with Si. In the solution cell containing 1 wt% NaOH, Si has strongly dissolved and an increased oxide component of Si.

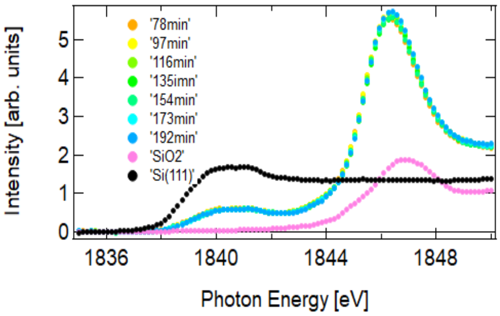

Fig. 1 XAFS spectra for Si in 1 wt% NaOH aqueous solutions.

Figure 2 depicts the XAFS spectra obtained from solution cells containing NaOH aqueous solutions with concentrations of 0.9 wt% along with Si. In the solution cell containing 0.9 wt% NaOH, Si gradually dissolves, accompanied by a slight increase in the oxide component of Si, indicating an intermediate reaction state.

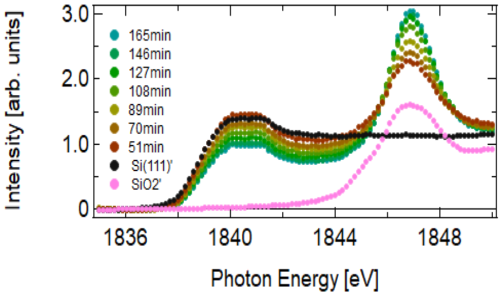

Fig. 2 XAFS spectra for Si in 0.9 wt% NaOH aqueous solutions.

As clearly shown in Fig. 3, the peak position corresponding to Si's tetravalent state shifts as the reaction progresses.

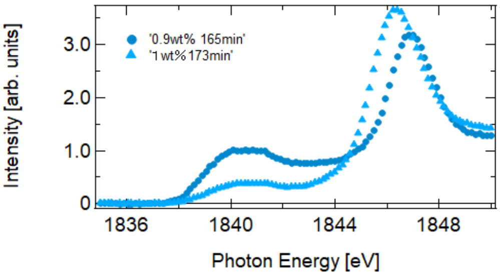

Fig. 3 Comparison of XAFS spectra for Si in 1 wt% and 0.9 wt% NaOH aqueous solutions.

References

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[3] S. Nishimura, S. Fujimura, K. Mitsuhara, M. Takizawa, and E. Yamasue, *MEMOIRS OF THE SR CENTER RITSUMEIKAN UNIVERSITY*, **2020**, 22, 49.