# 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 [1-4]. 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 solutions 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. The XAFS measurements for reference samples of Si, $SiO_2$, and $Na_2SiO_3$ were also carried out. 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. Spectral analysis indicates that $Na_2SiO_3$, $SiO_2$, and Si components are present during the reaction of Si with 1 wt% NaOH solution.

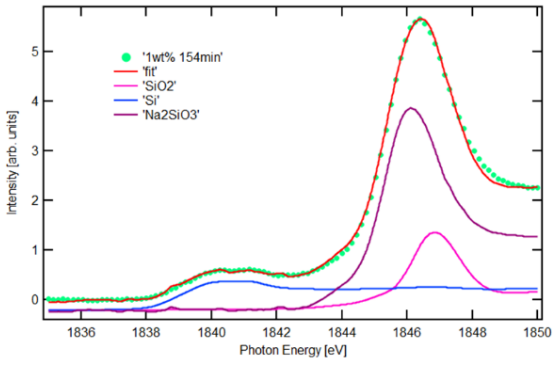


**Fig. 1** XAFS spectral analysis for Si in 1 wt% NaOH aqueous solution.

Figure 2 depicts the XAFS spectra obtained from solution cells containing NaOH aqueous solutions with concentrations of 0.09 wt% along with Si. Spectral analysis indicates that $SiO_2$ and Si components are present during the reaction of Si with 0.09 wt% NaOH solution.

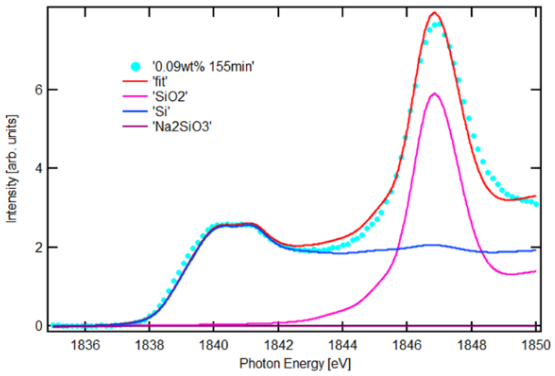


**Fig. 2** XAFS spectral analysis for Si in 0.09 wt% NaOH aqueous solution.

Depending on the NaOH concentration, reaction product is found to be different. For the low NaOH concentration (~0.09 wt%), main product of $SiO_2$ is the results of the following reactions:

$$Si + 2OH^- \rightarrow SiO_2 + H_2 + 2e^-$$
$$2H_2O + 2e^- \rightarrow H_2 + 2OH^-.$$

For the high NaOH concentration (~1 wt%), additional product of $Na_2SiO_3$ is the results of the following additional reaction:

$$Si + 2NaOH + H_2O \rightarrow Na_2SiO_3 + 2H_2.$$

## References

[1] Shugo Nishimura, Shiho Fujimura, Kei Mitsuhara, Masaru Takizawa, and Eiji Yamasue, MEMOIRS OF THE SR CENTER RITSUMEIKAN UNIVERSITY **22**, 49 (2020).
[2] Shoki Kosai, Shiho Fujimura, Shugo Nishimura, Shunsuke Kashiwakura, Kei Mitsuhara, Masaru Takizawa, and Eiji Yamasue, Int. J. Hydrogen Energy **46**, 7722 (2021).
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