Local Structure Analysis of Non-Crystalline Materials based on PDFs

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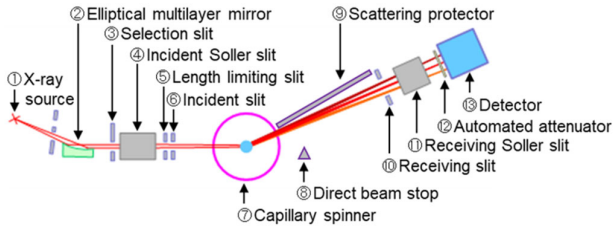
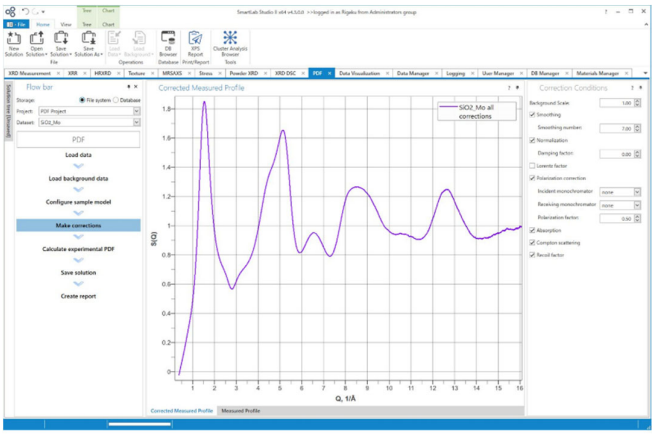
Experimental and analysis details

Using the SmartLab system, we obtained high-quality scattering patterns for PDF analysis. We used a high-power PhotonMax 9 kW rotating anode X-ray source with Ag target and CBO-E elliptical multilayer mirror for Ag radiation to condition a high-resolution focusing beam. A scattering protector and a 2.5-deg Soller slit were used in the receiving optics to eliminate parasitic scattering from the incident optics and air. We also used a D/teX Ultra HE 1D detector as a high-efficiency detector for the high-energy X-ray source to collect data rapidly.

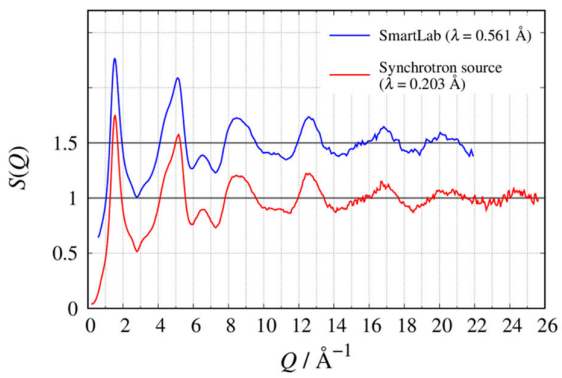


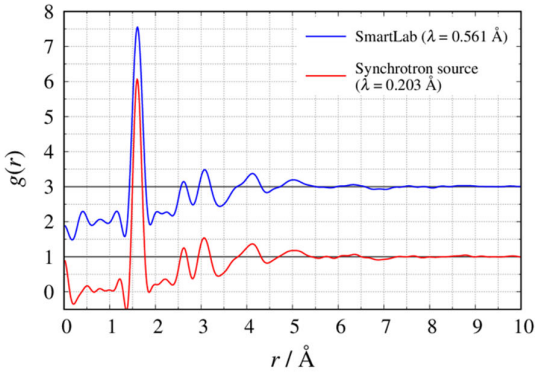


SmartLab Studio II PDF plugin

Experimental results in comparison with synchrotron results

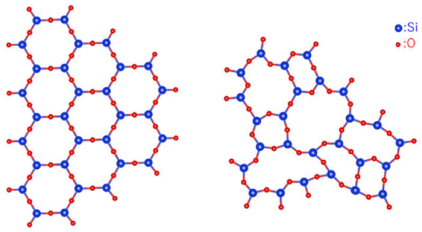
We used the Ag Kα wavelength source to collect as high-q data as possible. Compared to the structure factors from the experimental results from a synchrotron facility, we obtained almost the same S(Q) pattern using SmartLab. As a result, the calculated PDF based on the results from SmartLab were quite similar to that from a synchrotron facility.





Structure analysis of SiO_2 and its derivatives based on experimental PDFs

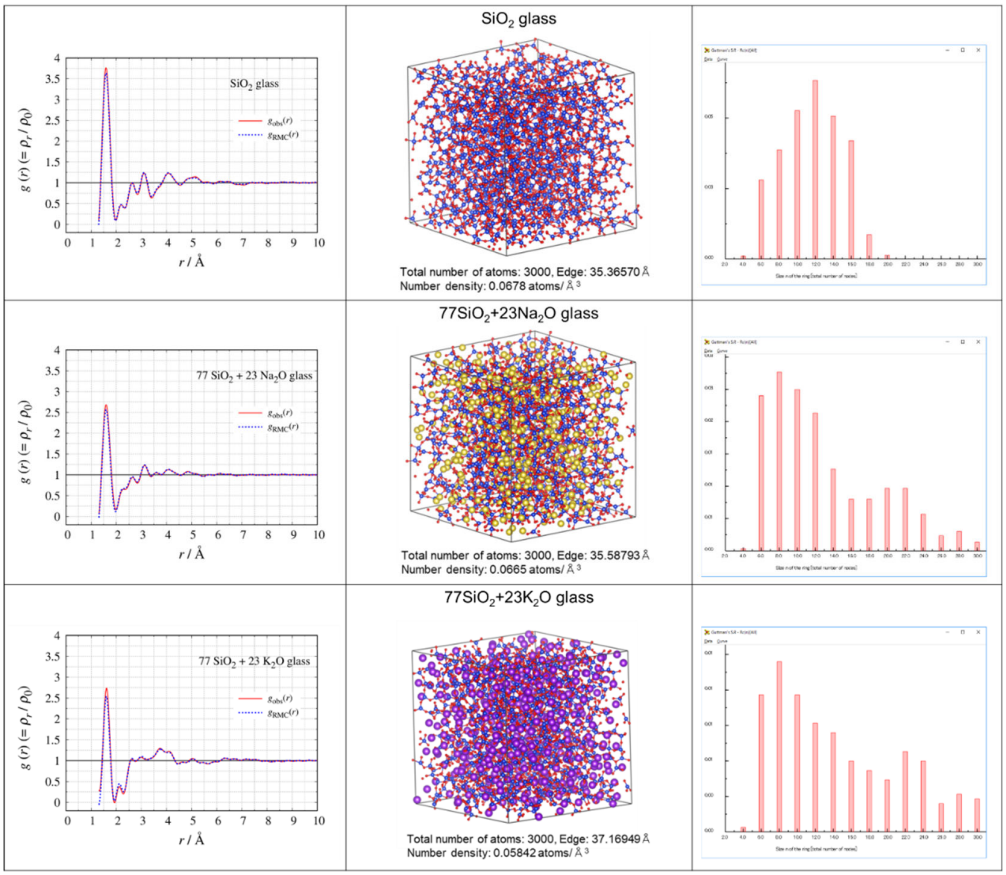
Using the SmartLab system, we collected scattering patterns of noncrystalline SiO_2 and its derivatives ($77SiO_2$+$23Na_2O$, $77SiO_2$+$23K_2O$). Based on the scattering patterns, the PDF of each compound was calculated. Based on the obtained PDFs, the structure of each compound was analyzed using a reverse Monte Carlo algorithm (RMC Profile software[1]). Each structural model well reproduced the corresponding experimentally obtained PDF.



Local structure of rings in crystalline (left) and amorphous silica (right)

Then, the numbers of *n*-membered rings existing in each structure were counted using the ISAACS software[2,3].

In the case of SiO_2, 12-membered rings were the most probable[4] and rings larger than 20-membered were not observed. In the cases of Na,K+SiO_2, 8-membered rings were the most probable and rings larger than 20-membered were also observed for both cases. This indicates that Si/O rings became larger due to the incorporation of sodium/potassium ions into them.



References

(1) R. L. McGreevy *et al.*, *Molecular Simulation*, **1**, 359-367(1988).
(2) S. Le Roux and V. Petkov: *J. Appl. Cryst.*, **43** (2010), 181-185.
(3) L. Guttman: *J. Non-Cryst. Solids*, **116** (1990), 145-147.
(4) S.Kohara *et al.*, *Proc. Nat.Acad.Sci.,* **108(36)**, 14780(2011).