Damage-free 100-nm-localized coherent SAXS analysis of fuel cell catalysts using X-ray free-electron lasers

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The realization of a hydrogen society, where hydrogen serves as a clean and renewable energy source, is desired to reduce carbon dioxide emissions and achieve sustainable development. Polymer electrolyte fuel cells (PEFCs) are a key technology for automobiles in the hydrogen society. This study aims to analyze the nanostructures of the catalyst inks of PEFCs. In the catalyst layer, catalyst nanoparticles are supported on carbon and are thinly covered with an ionomer that facilitates proton conduction. We are particularly interested in examining the ionomer coating, which is important for PEFCs' performance but has been difficult to analyze.

We conducted coherent small-angle x-ray scattering (SAXS) measurements on PEFC catalyst inks using an 100-nm focused X-ray free-electron laser (XFEL) beam [1] with a photon energy of 4 keV at SACLA. The femtosecond XFEL pulses allowed us to perform radiation-damage-free measurements by outrunning major radiation-damage processes. Such damage-free measurements are highly valuable because radiation damage often poses challenges in high-resolution observation of ionomers using X-rays and electron beams. The measurements wer carried out for catalyst inks in both dried and solution states. The dried sample was prepared by dropping catalyst ink onto a silicon nitride membrane and air-drying it. The solution sample was enclosed in micro-liquid enclosure arrays [2] developed at Hokkaido University.

Experimental coherent SAXS data revealed contributions from the ionomer [3], which were previously thought to be difficult to capture due to strong X-ray scattering from the catalyst nanoparticles. Moreover, femto-second single-shot coherent SAXS data suggested spatial hetero-geneity in ionomer coating. To interpret the experimental data, we also performed simulations (Fig. 1) using an all-atom model based on reaction molecular dynamics calculations. To our knowledge, SAXS simulation on PEFC catalysts using an atomic model has notr been reported previously.

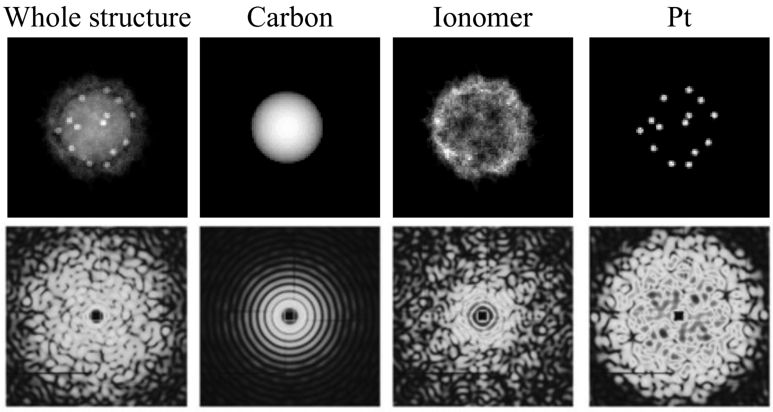

Figure 1: Simulation of coherent SAXS patterns (lower panel) of each component of catalyst ink (upper panel) using all-atom molecular dynamics calculation model.

References

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