Preliminary neutron diffraction study of high-potential iron-sulfur protein at J-PARC

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The redox states of high-potential iron-sulfur protein (HiPIP) have been reported to be stabilized by solvent molecules around the protein surface [1]. Information about hydrogen atoms is required to determine the orientation of solvent molecules, especially that of water molecules. X-ray crystal structures of HiPIP determined at ultra-high resolutions include hydrogen atoms of amino acid residues and those of some water molecules [2]. However, significant structural changes were not observed between oxidized and reduced forms of HiPIP. We have performed neutron diffraction experiment of HiPIP at iBIX beamline of J-PARC to obtain structural information about hydrogen atoms that have not been observed in the X-ray crystal structures.

The crystal of the oxidized form of HiPIP was obtained by macro-seeding method and the size of the crystal was reached to 1 mm^3. The crystal was soaked in deuterated solution for 3 months, and then the crystal was transferred to cryoprotectant solution for data collection at 100 K. Concentration of the protectant solution was gradually increased not to deteriorate diffraction power of the crystal. The crystal was flash frozen in a nitrogen-gas stream at 100 K and it was cooled during the data collection. Diffraction spots were observed up to 1.1 Å resolution after exposure to neutrons for 9 hours. The diffraction data is the highest resolution in the neutron diffraction data of the protein crystals [3].

References

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