Poster Presentation

MS22.P30

X-Ray Diffraction of Magnetically Oriented Microcrystals of Protein

S. Tsukui[1], F. Kimura[1], K. Mizutani[2], B. Mikami[2], T. Kimura[1]

[1]Kyoto University, Graduate School of Agricultur, Kyoto, Japan, [2]Kyoto University, Graduate School of Agricultur, Uji, Japan

Elucidation of the three-dimensional structure of biomolecules is of great importance because the three-dimensional structure is closely related to biological functions. X-ray single-crystal analysis is powerful method to analyze the structure, but it is sometimes difficult to grow a crystal sufficiently large for conventional or even synchrotron single-crystal X-ray measurement. We recently reported on a magnetically oriented microcrystal array (MOMA) [1] that is a composite in which microcrystals are aligned three-dimensionally in polymer matrix. Microcrystals are suspended in an ultraviolet-curable monomer and rotated non-uniformly in a static magnetic field to achieve three dimensional crystal alignment. Then, the monomer is photopolymerized to maintain the achieved alignment. We have successfully demonstrated that X-ray single crystal structure determinations through MOMA are possible for low molecular weight compounds [2] as well as protein. [3] However, the method with MOMA has two drawbacks: (i) the sample microcrystals cannot be recovered from a MOMA, which is especially serious problem in case of proteins, and (ii) the alignment is deteriorated during the consolidation process, causing low resolution. In this study, we attempt to solve these problems. First, we use a water-soluble sol as microcrystalline media and consolidate the alignment by gelation, which makes the recovery of microcrystals possible. Second, a magnetically oriented microcrystal suspension (MOMS) is used for in-situ X-ray diffraction measurement, which makes the sample recovery possible and enhances the resolution. We use lysozyme as a model protein for both cases. The in-situ method with in-house X-ray diffractometer gave diffraction spots about 3.0 Å resolutions. We plan to perform the same experiment at SPring-8.

[1] *T. Kimura, F. Kimura, and M. Yoshino, Langmuir 22 (2006) 3464-3466.,* ***[2]*** *F. Kimura, T. Kimura, W. Oshima, et al., J. Appl. Crystallogr., 43 (2010) 151-153.,* ***[3]*** *F. Kimura, K. Mizutani, B. Mikami, et al., Cryst. Growth Des. 11 (2011) 12-15.*

Keywords: Protein microcrystal, Magnetic alignment, Structure analysis