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In order to elucidate the intermolecular interactions involved in complex formation of chitosan with hydrogen halides, crystal structures of chitosan complexes with HBr and HI were analyzed based on synchrotron X-ray fiber diffraction data (BL40B2, SPring-8, Hyogo, Japan). Both crystals are isomorphous and belong to the monoclinic space group $P2_1$. The unit cell constants are a = 9.299(9), b = 9.504(8), c(fiber axis) = 10.41(1) Å and beta = 106.93(8) deg, and a = 9.46(2), b = 9.79(2), c(fiber axis) = 10.33(2) Å and beta = 105.1(2) deg for HBr and HI complexes, respectively. The final packing models were obtained by the linked-atom least-squares refinement, which gave R-factors of 0.192 for HBr complex (93 observed spots) and 0.193 for HI complex (44 observed spots). The halide ions are aligned along the c-axis at intervals of about 5Å and are surrounded by four polymer chains. In an asymmetric unit, there are two halide ions. One ion accepts three hydrogen bonds from NH_3^+ groups (N2 nitrogen). The other one participates in one hydrogen bond from N2 and two hydrogen bonds from primary hydroxyl groups (O6 oxygen). In addition, the chitosan chains are linked by N-H...O and C-H...O hydrogen bonds along the b-axis direction. The crystal structure of the hydrated form of chitosan was reanalyzed using synchrotron X-ray fiber diffraction data (BL38B1, SPring-8). The chitosan chains make sheet structures parallel to the bc-plane and these sheets stack along the a-axis. Water molecules form columns between these sheets. The sites of the halide ions in the complex crystals are similar to those of the water molecules in the hydrated form. It was suggested that the columnar structure of water in the hydrated form plays an important role for the complex formation.

Keywords: complexes, fibre diffraction, synchrotron radiation

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Structural analysis of F-actin using fiber diffraction

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Actin is on of the most abundant protein and works in the eukaryotic cells. Actin has two state－monomeric G-actin and polymerized F-actin. The F-actin is a functional form in muscle and cellar transportation. Also the processes of polymerization of actin are important for cell motility. In 1990, crystal structure of actin-DNase I complex was solved by Holmes group. Since then, a lot of crystal structures of actin were solved. Actin has a nucleotide-binding cleft enclosed by two major domains. In almost all of actin crystal structure, the cleft is closed and the two domains are tilted each other in the propeller-like manner. The conformation appears to be typical G-actin conformation. In the back-to-back paper, his group also proposed the structural model for F-actin using the fiber diffractions from well-oriented sols. The monomer arrangement and orientation in the F-actin model have widely been accepted. However, to precede the next steps of actin studies, for example detailed interaction between F-actin and myosin, actin ATPase and polymerization, we need a precise model for the F-actin structure. We recorded the diffraction patterns from well-oriented F-actin sols at SPring-8. Using the diffraction pattern up to 3.3 Å resolution in the radial direction and 5.5 Å along the equator, we made a new model for F-actin structure. We put crystal structures in helical arrangement of F-actin and fitted the model to the reflection data using a combination of normal mode motions of G-actin. After that, we refined the structure using the MD refinement by FX-plor. We found a novel conformation of actin in F-actin filament. In this conformation, whole molecule is flat and the nucleotide binding cleft remains closed.

Keywords: actin, fiber diffraction, macromolecular polymer

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Computational methods in fibre diffraction

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Fibre diffraction is used in structure determination of filamentous biological polymers when conventional macromolecular crystallography cannot be applied. The technique made a critical impact in the early days of structural biology, but since then has gone largely unheralded, partially owing to the limitations of available computational tools. With the advancement of computer and synchrotron technologies and the arrival of new structural problems, creating reliable software for fibre diffraction research became both feasible and urgent. In collaboration with fibre diffraction communities in North America and Europe, we have developed and integrated a collection of such software tools. These tools include WCEN for analysis of diffraction patterns, correcting systematic effects and mapping diffraction data into reciprocal space, RAD for angular deconvolution of diffraction data from partially oriented specimens, FX-PLOR for model building and refinement against high resolution diffraction data, and FNV for analysis using Fourier-Bessel transforms and syntheses. The software collection, already successfully applied in the study of non-crystalline filamentous systems such as amyloids and viruses, together with the CCP13 software suite, covers all aspects of fibre diffraction. The work is supported by FiberNet, a Research Coordination Network for Fiber Diffraction from Biological Polymers and Assemblies established through NSF grant MCB-0234001.

Keywords: fibre diffraction, macromolecular structure determination, computational method

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Application of neutron imaging plate system to crystal structure analysis of deuterated polymers

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The 2-dimensional neutron imaging plate system BIX-3, develped for the structural biology, has been succesfully applied to the crystal structure analysis of various kinds of synthetic polymers, and the extraction of hydrogen atom positions has been made with high accuracy. The polymers investigated here were polyethylene, polyoxymethylene, isotactic polypropylene, poly(ethylene oxide),