MS13.03.06 STRUCTURE ANALYSIS OF HYDRATED CHITOSAN BY UTILIZING IMAGING PLATE. By K. Okuyama, K. Suzuki, Y. Obata, T. Yui* and K. Ogawa**, Tokyo University of Agriculture and Technology, Koganei, Tokyo 184, Japan, *Miyazaki University, Miyazaki 889-21, Japan and **University of Osaka Prefecture, Sakai, Osaka 593, Japan.

The molecular and crystal structure of the hydrated chitosan derived by deacetylation of chitin tendon was determined by the X-ray diffraction method and a linked-atom least-squares technique. The X-ray intensities were measured using the imaging plate. The data processing and structure analysis were done using an inhouse software developed recently (Okuyama, K., Obata, Y., Noguchi, K., Kusaba, T., Ito Y. and Ohno, S., Biopolymers, 1996, **38**, in press.). The crystals of the polymer chains belong to the orthorhombic system, space group $P2_12_12_1$ with a=8.91(4), b=16.87(6) and c (fiber axis) =10.34(4)Å. The unit cell contains eight monomer residues and eight water molecules. Since the polymer chain has a 2_1-helical symmetry, four chains are included in a cell.

The molecular chain is stabilized by an intramolecular O3—O5 hydrogen bond similar to those found in many β(1→4) linked polysaccharides and has a *gt* conformation for the hydroxymethyl moiety at C5 atom. Polymer chains arranged in an antiparallel fashion are connected by an intermolecular NH—O6 hydrogen bond and a hydrogen bond bridge through water molecule, making a sheet structure along the *b*-axis. These sheets are stacked along the *a*-axis and are connected by hydrogen bond bridges through the second water molecule. The final X-ray residuals are R=0.185 and R"=0.194.

In the crystal structure of anhydrous form of chitosan (Yui, T., Imada, K., Okuyama, K., Obata, Y., Suzuki K. and Ogawa, K., Macromolecules, 1994, **27**, 7601), parallel chains make a sheet structure by an intermolecular NH—O6 hydrogen bond. Therefore, the transition from the hydrous to the anhydrous form needs cleavage of the NH—O6 hydrogen bond between antiparallel molecular chains and the formation of the new NH—O6 bond between parallel polymer chains.

MS13.03.07 X-RAY DIFFRACTION EVIDENCE THAT CROSSBRIDGES WEAKLY BOUND TO ACTIN IN MUSCLE ARE DISORDERED (NONSTEREOSPECIFIC BINDING). L.C. Yu+, S. Xu+, S. Malinchik+, T. Kraft+ and B. Brenner*. +NIAMS, NIH; *Hannover Medical School, Hannover, Germany

Generation of isometric force, different from quick tension recovery, was proposed to result from a structural change in the actomyosin (cross bridge) complex associated with the transition from a weakly bound configuration to a strongly bound configuration (Brenner, et al., 1995). Structurally, we proposed that the weak to strong transition is from nonstereospecific attachment to stereospecific attachment. Recently we have systematically obtained two dimensional X-ray diffraction patterns from skinned rabbit psoas fiber bundles, relaxed and in rigor, such that direct quantitative comparisons can be made. (Data obtained on EMBL beamline X-13 at DESY). For 4°C and 20°C, and ionic strength 50-150 mM, under relaxing condition, at least 6 orders of thick filament based layer lines are visible. Analysis of the axial centroid position of the inner region of the first layer line suggests that the layer line is a mixture of overlapping thick and thin filament based layer lines and their relative contribution varies with ionic strength, correlating with the fraction of weakly bound crossbridges. The behavior of the mixed layer line could be explained by modeling attachment of myosin heads to specific sites on actin while the binding angle is variable. Another evidence of nonstereospecific binding is that the diffuse scattering is little affected by considerable change in the fraction of weakly bound cross-bridges as ionic strength is changed; i.e. the weakly bound cross-bridges are disordered. As a comparison, in transition from relaxed condition to rigor where the cross-bridge attachment is known to be stereospecific, the diffuse background decreases significantly. The results support the idea that the weakly attached cross-bridges assume nonstereospecific conformations.

Some of the cross bridges that are not attached to actin form a helix around the backbone of the thick filament. The helical structure is highly sensitive to temperature. Results of the analysis and modelling will be presented. (NATO grant 930448; DFG Br849/1-4).

MS13.03.08 BACKGROUND CORRECTION OF NEUTRON AND X-RAY FIBER DIFFRACTION DATA. Ivanova, M. and Makowski, L., Chemistry Department, Florida State University, Tallahassee, FL 32306-3006, USA

Background estimation is the limiting factor in processing of fiber diffraction data. Background in fiber diffraction pattern is not readily measurable except at resolution low enough that adjacent layer lines do not overlap. Estimation at larger diffraction angles is problematic since there is no way to reliably identify a point on the pattern where the only contribution is the background. Where this positions can be identified, it is possible to estimate the background by fitting the observed background points to a set of cylinder functions, A parameterization of the background can also be integrated to estimation of the layer line intensities bay angular deconvolution. This works for cases where the background can be well represented by a limited number of cylinder functions. To address the more general problem we used the observation that the spatial frequencies making up the background are much lower than those that constitute the data, and used iterative low pass filtering to separate the contributions from the layer line data and from the background. This process has been integrated into angular deconvolution to provide accurate estimates for data from x-ray and neutron diffraction patterns that could not be successfully processed by previous methods. We have applied the method successfully to x-ray diffraction patterns from mutant filamentous bacteriophage fddx and neutron diffraction patterns from specifically deuterated M13 phage particles.