

P12.11.50

Acta Cryst. (2008). A64, C562**In-plane stress and strain components of epitaxially grown Zn:LiNbO₃ thin films**Juergen Kraeusslich¹, Carsten Dubs², Andreas Lorenz², Andreas Tuennermann¹¹University Friedrich Schiller, Max-Wien-Platz 1, Jena, Germany, 07743, Germany, ²INNOVENT, Pruessingstrasse 27B, 07745 Jena, Germany, E-mail: kraeusslich@ioq.uni-jena.de

As a precursor material for electrooptical applications in the integrated optics, undoped as well as Zn-doped stoichiometric LiNbO₃ thin films of a few μm thickness were grown by high-temperature liquid phase epitaxy on congruent LiNbO₃ substrates. The crystalline perfection and lattice parameters of the epitaxially grown thin films were investigated by means of high-resolution x-ray diffraction methods. From the symmetrical $\theta/2\theta$ -diffractograms (Fig. 1) a lattice parameter change results perpendicular to the sample surface of $(\delta d/d)$ up to 10^{-3} with increasing Zn content. Despite different Zn contents, the Zn-substituted LiNbO₃ thin films reveal a distinctly pseudomorphous growth. Using the generalized Hooke's law in matrix way of writing and taking the measured values into account, the relaxed lattice parameters of the grown thin films as well as the in-plane strain and tension components of the Zn:LiNbO₃ thin films have been numerically calculated.

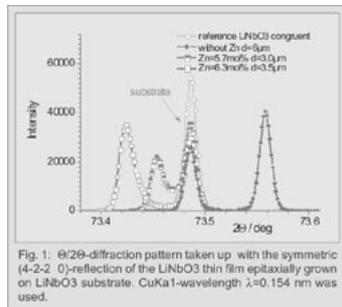


Fig. 1: $\theta/2\theta$ -diffraction pattern taken up with the symmetric (4-2-2 0)-reflection of the LiNbO₃ thin film epitaxially grown on LiNbO₃ substrate. CuK α 1-wavelength $\lambda=0.154$ nm was used.

Keywords: lithium niobate, thin films, X-ray strain determination

P13.03.01

Acta Cryst. (2008). A64, C562**Orientation of myosin crossbridges obtained by X-ray fiber diffraction from relaxed skeletal muscles**Kanji Oshima¹, Yasunobu Sugimoto², Katsuzo Wakabayashi²¹Osaka University, The center for advanced medical engineering and informatics, 2-2, Yamadaoka, Suita, Osaka, 565-0871, Japan, ²Osaka University, 1-3, Machikaneyama-cho, Toyonaka, Osaka, 560-8531, Japan, E-mail: oshima@protein.osaka-u.ac.jp

A new method for eliminating a partial sampling effect due to the hexagonal lattice of myofilaments on the layer-line intensities in X-ray diffraction patterns from muscles at full-overlap between the thin and thick filaments was developed using the cylindrically averaged Patterson function. We validated the new method in the computational calculation using thick filament models with two different axial periodicity of the crossbridge arrangement previously reported (Oshima et al., *JMB* 367, 275-301 (2007)) and applied it to the intensity analysis of myosin-based layer lines from relaxed muscles with the full-filament overlap. Using the corrected intensity data we carried out the modeling analysis on azimuthal orientation of two heads of a myosin crossbridge and compared the optimum model to that from muscles at the non-overlap filament length previously reported (Oshima et al., *JMB* 367, 275-301 (2007)). The result reveals that the configuration of myosin heads in the regular repeating region of crossbridges is similar to that in muscles at the non-overlap length but it is somewhat different in the perturbed

repeating region of crossbridges. In the regular region one myosin head of a crossbridge sits in the close vicinity to another head in a pair at an adjacent crown level along the filament axis. In the perturbed region, one head of a myosin crossbridge seems to be in contact with the other head at the same axial crown level. Our modeling analysis suggests that the dispositions of two-headed crossbridges are stabilized by the interaction between two heads at the same or different axial levels rather than by an electrostatic balance between the thick and thin filaments.

Keywords: Patterson method, myosin, synchrotron X-ray diffraction

P13.03.02

Acta Cryst. (2008). A64, C562**Structural changes of myofilaments in live frog skeletal muscle caused by double pulse stimulation**Tatsuhito Matsuo^{1,2}, Naoto Yagi¹¹SPring-8/JASRI, tatsu@spring8.or.jp, Sayo, Hyogo, 679-5148, Japan, ²Osaka University, E-mail: tatsu@spring8.or.jp

Skeletal muscle has a quasi-crystalline order of proteins. Thus, it is possible to observe structural changes of contractile and regulatory proteins in a muscle under physiological conditions. Live muscle produces transient tension by a single electrical stimulus and more tension develops by a second stimulus, while intracellular free calcium concentration is not summed significantly. In this study, to investigate the structural changes of myofilaments caused by the double pulse stimulation, the Small-Angle X-ray Diffraction (SAXD) patterns from a live frog skeletal muscle were recorded at a time resolution of 1 msec using SPring-8. The separation of the pulses was 15 msec. From the analysis of the SAXD patterns following results were obtained: the intensity of the meridional myosin-related reflections at $1/21.5$ nm⁻¹ and $1/14.3$ nm⁻¹ and that from C-protein (MyBP-C) at $1/44.1$ nm⁻¹ dropped drastically with the first stimulus, showing that the ordered array of myosin-heads and C-protein was disordered considerably by the first stimulus. The intensity drop of the equatorial (1,0) reflection from the hexagonal filament lattice was larger with the second stimulus, showing that more cross-bridges are formed. The intensity of the meridional troponin-related reflections at $1/38.5$ nm⁻¹ showed a biphasic change with the first stimulus, and the maximum amount of intensity change was not affected significantly by the second stimulus, indicating that the thin filament structure was changed cooperatively by attachment of a small number of myosin heads. These results indicate that the regulatory system in the thin filament has a highly cooperative nature and both the thin and the thick filaments undergo large structural changes with the first stimulus

Keywords: muscle time-resolved X-ray diffraction, fibre diffraction, muscle contraction

P13.03.03

Acta Cryst. (2008). A64, C562-563**Neutron fiber diffraction measurements of muscle using the contrast variation technique**Satoru Fujiwara¹, Yasunori Takezawa², Yasunobu Sugimoto², Katsuzo Wakabayashi²¹Japan Atomic Energy Agency, Quantum Beam Science Directorate, 2-4 Shirakata-Shirane, Tokai-mura, Naka-gun, Ibaraki, 319-1195, Japan, ²Division of Bioengineering, Graduate School of Engineering Science,

Osaka University, Toyonaka, Osaka 560-8531, Japan, E-mail : fujiwara.satoru@jaea.go.jp

Among various methods for structural studies of biological macromolecules, neutron scattering and diffraction have a unique feature that the contrast between the scattering length density of the molecules and that of the solvent can be varied easily by changing D₂O content in the solvent. This “contrast variation” technique enables it to obtain information on internal fluctuations or a variation of scattering length density of the molecules of interest. Here, in order to explore the possibilities of neutron fiber diffraction, the contrast variation technique was applied to measurements of neutron fiber diffraction of muscles. The neutron fiber diffraction patterns of frog sartorius muscles were measured under the relaxed state where no tension of the muscle is produced, and under the rigor state where the myosin heads of the thick filaments bind tightly to actin in the thin filaments, in various D₂O concentrations. It was shown that under both states, there were reflections having distinct contrast matching points, indicating a variation in the scattering length density distribution in the unit cell of the muscle structure. Analysis of the equatorial reflections showed that the phase information of these reflections is obtained, that the density projected to a plane perpendicular to the axis of the muscle is different between the thick filament region and the thin filament region, and that the projected density of the thick filament changes as the state of the muscle changes from the relaxed state to the rigor state. Analysis of the meridional reflections of the thick filament suggested that in addition to contributions from the myosin head regions, the backbone region of the thick filaments contributes to the intensity of the meridional reflections as well.

Keywords: fibre diffraction, muscle, neutron diffraction

P13.03.04

Acta Cryst. (2008). A64, C563

Molecular orientation of a collagen hydrogel with high mechanical strength

Chizuru Hongo^{1,2}, Michiya Matsusaki^{1,2}, Kohji Nishida³, Mitsuru Akashi^{1,2}

¹Osaka University, Department of Applied Chemistry, Graduate School of Engineering, 2-1 Yamadaoka, Suita, Osaka, 565-0871, Japan, ²21st Century COE Program, CICET, Osaka University, ³Tohoku University Graduate School of Medicine, 1-1 Seiryomachi Aoba-ku, Sendai, Miyagi 980-8574, E-mail : chizuh@chem.eng.osaka-u.ac.jp

Collagen is a major fibrous protein of the extracellular matrix. The molecule has a triple-helical structure and is known to assemble to form fibrils. Furthermore, collagen fibrils organized into one direction to form fibers in tendons and ligaments. The orientation of these molecules is known to be a significant factor in the mechanical strength of natural tissues such as bone, tendon, ligament and the cornea. Accordingly, the construction of collagen gels with oriented fibrils attracts much attention for tissue engineering. We reported a novel and simple method to prepare collagen gels with molecularly oriented fibrils. In this study, x-ray diffraction measurements

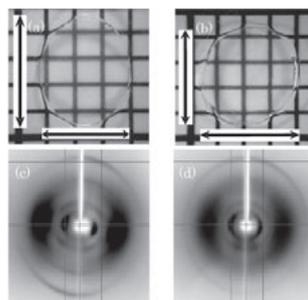


Fig. 1 Optical photomicrographs and X-ray diffraction patterns of oriented (a and c) and non-oriented (b and d) collagen gels, respectively.

were performed to confirm the molecular orientation in the gels. Amazingly, the pattern of oriented gel was quite similar to that of native tendon collagen, which shows narrower arc pattern than that of non-oriented gel (Fig.1). The results of the diffraction patterns clearly suggested a highly-ordered molecular orientation of the fibrils in the oriented gels. We succeeded in the controlling of the orientation of the fibrils in the gel. This technique is considerably effective as the regenerative medicine technology.

Keywords: collagen, fibre diffraction, molecular orientation

P13.03.05

Acta Cryst. (2008). A64, C563

Multiple scattering of light by collagen nanofibres in biological tissues

Siranush E. Bezirganyan, Greta R. Ulikhanyan

Yerevan State Medical University after Mkhitar Heratsi, of Medical & Biological Physics, 2, Koryuni Street, Yerevan, Yerevan Distr., 0025, Armenia, E-mail : sira_be@yahoo.com

Some biological tissues look like a fibrillar texture, which can provide an intense response to incident electromagnetic waves. This gives the possibility to perform investigations of optical properties and structure of such natural textures. Natural collagen fibrils are encountered, for example, in the cornea and sclera. Both cornea and sclera tissues are essentially binary nano-composite materials, consisting of collagen fibrils embedded in a water-based mucopolysaccharide background substance, whose refractive index is different from the refractive index of collagen fibres. It is well known (e.g. see [1]) that difference in the structure of cornea and sclera is governed by the arrangement and sizes of collagen fibrils in the background substance, which makes such a difference in the optical performance of the transparent cornea and the opaque sclera. Here we explain optical properties of cornea and sclera by 2D quasi-crystalline lattice model constructed from rods (fibres) of dielectric constant infinite in one direction. Bloch proved in 1928 that waves in periodic media can propagate without scattering, their behaviour governed by a periodic envelope function multiplied by a plane wave [2]. This technique can be applied to electromagnetism by considering Maxwell's equations as an eigenvalues and eigenfunctions problem in analogue with Schrödinger's equation (e.g. see [3, 4]). Such approach to considered model of quasi-periodic fibrillar texture takes into account a multiple scattering of light by collagen fibres.

[1] Komai Y. and Ushiki T., *Invest. Ophthalmol. Vis. Sci.* 1991, 32, 2244.

[2] Bloch F., *Ann. École Norm. Sup.*, 1928, 55, 555.

[3] Bezirganyan H.P., Bezirganyan P.H., *Phys. Stat. Sol. (a)*, 1988, 105, 345.

[4] Bezirganyan H.P., *Phys. Stat. Sol. (a)*, 1988, 109, 101.

Keywords: fibre diffraction theory, electromagnetic wave theory, quasicrystal scattering

P13.03.06

Acta Cryst. (2008). A64, C563–564

Crystal structures of chitosan and its complexes with hydrogen halides

Keiichi Noguchi¹, Masahisa Wada², Kenji Okuyama³, Kozo Ogawa⁴

¹Tokyo University of Agriculture & Technology, Instrumentation Analysis Center, Naka-cho 2-24-16, Koganei, Tokyo, 184-8588, Japan, ²The University of Tokyo, Bunkyo-ku, Tokyo 113-8657, Japan, ³Osaka