

**P12.11.50***Acta Cryst.* (2008). A64, C562**In-plane stress and strain components of epitaxially grown Zn:LiNbO<sub>3</sub> thin films**Juergen Kraeusslich<sup>1</sup>, Carsten Dubs<sup>2</sup>, Andreas Lorenz<sup>2</sup>, Andreas Tuennermann<sup>1</sup><sup>1</sup>University Friedrich Schiller, Max-Wien-Platz 1, Jena, Germany, 07743, Germany, <sup>2</sup>INNOVENT, 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 LiNbO<sub>3</sub> thin films of a few  $\mu\text{m}$  thickness were grown by high-temperature liquid phase epitaxy on congruent LiNbO<sub>3</sub> 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 LiNbO<sub>3</sub> 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:LiNbO<sub>3</sub> thin films have been numerically calculated.

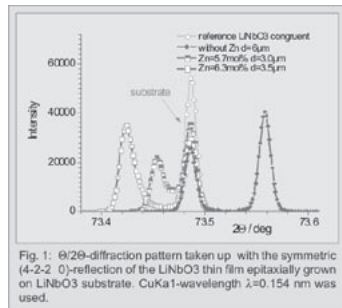


Fig. 1:  $\theta/2\theta$ -diffraction pattern taken up with the symmetric (4-2-2 0)-reflection of the LiNbO<sub>3</sub> thin film epitaxially grown on LiNbO<sub>3</sub> substrate. CuK $\alpha$ 1-wavelength  $\lambda=0.154$  nm was used.

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 Oshima<sup>1</sup>, Yasunobu Sugimoto<sup>2</sup>, Katsuzo Wakabayashi<sup>2</sup><sup>1</sup>Osaka University, The center for advanced medical engineering and informatics, 2-2, Yamadaoka, Suita, Osaka, 565-0871, Japan, <sup>2</sup>Osaka 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<sup>1,2</sup>, Naoto Yagi<sup>1</sup><sup>1</sup>SPring-8/JASRI, tatsu@spring8.or.jp, Sayo, Hyogo, 679-5148, Japan, <sup>2</sup>Osaka 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<sup>-1</sup> and  $1/14.3$  nm<sup>-1</sup> and that from C-protein (MyBP-C) at  $1/44.1$  nm<sup>-1</sup> 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<sup>-1</sup> 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 Fujiwara<sup>1</sup>, Yasunori Takezawa<sup>2</sup>, Yasunobu Sugimoto<sup>2</sup>, Katsuzo Wakabayashi<sup>2</sup><sup>1</sup>Japan Atomic Energy Agency, Quantum Beam Science Directorate, 2-4 Shirakata-Shirane, Tokai-mura, Naka-gun, Ibaraki, 319-1195, Japan, <sup>2</sup>Division of Bioengineering, Graduate School of Engineering Science,