Biological Science

15A/2005G310

The Deduction of a Single Filament Transform from Partially Sampled Myosin-based Layer Lines in X-ray Diffraction Patterns from Resting Skeletal Muscles

Kanji OSHIMA[1], Yasunori TAKEZAWA[2], Yasunobu SUGIMOTO[3], and Katsuzo WAKABAYASHI*[3]
[1]The cent. for Adv. Med. Eng. and Info., Osaka Univ., Suita, Osaka 565-0871, Japan
[2]Div. of Chem. Eng. Sci., Grad. Sch. of Eng. Sci., Osaka Univ., Toyonaka, Osaka 560-8531, Japan
[3]Div. of Biophys. Eng., Grad. Sch. of Eng. Sci., Osaka Univ., Toyonaka, Osaka 560-8531, Japan

Introduction

There are partially but strong sampling effects on the myosin-based layer lines due to imperfect hexagonal arrays of myofilaments in X-ray diffraction patterns from resting skeletal muscles at full-filament overlap length. To investigate azimuthal orientations of each head of a double-headed myosin crossbridge around the filament axis, we have to correct these sampling effects on the layer lines. We have developed a method for correcting the sampling effects reported previously [1]. In this method we used a cylindrically averaged difference-Patterson function ($\Delta Q(r,z)$) [2] to calculate sampling-free layer-line intensities by removing appropriately distant peaks appeared in the $\Delta Q(r,z)$ map. We examined the validity of the method using a hexagonal-filament array model and a single filament model.

Modeling calculation

To examine the validity of the correcting method, we used two thick filament models to calculate the layer-line intensities; one of which consists of a single filament with the same azimuthal orientations of heads as those of the thick filament model reported previously [3] (referred to as a single filament model) and the other consists of four filaments forming a simple hexagonal filament array (referred to as a hexagonal-filament array model) (see Fig.1 A for an arrangement), where each filament has the same azimuthal orientation as that of a single filament model for the sake of simplicity. We calculated the $\Delta Q(r,z)$ map for each model and removed the outer peaks beyond the borderline ($r > 30$ nm) from the $\Delta Q(r,z)$ map of a hexagonal-filament array model to calculate the sampling-free layer-line intensities.

Results

Figure 1B shows the comparison of the corrected layer-line intensities of a hexagonal-filament array model with those of a single filament model. The corrected layer-line intensities have little sampling effect, very similar to those of a single filament model, indicating that this method eliminates mostly sampling effects due to the hexagonal filament array on the layer lines. We qualified the difference in the layer-line intensities between the two models using the *RMSI* (root mean square of intensity) described below.

$$RMSI = \frac{\sum_{i=1}^{6}\int_{0.0254}^{0.157}\left|I_{hexagonal,\,i}(R) - s_c I_{single,\,i}(R)\right|dR}{\sum_{i=1}^{6}\int_{0.0254}^{0.157} I_{single,\,i}(R)dR} \qquad s_c = \frac{\sum_{i=1}^{6}\int_{0.0254}^{0.157} I_{hexagonal,\,i}(R)dR}{\sum_{i=1}^{6}\int_{0.0254}^{0.157} I_{single,\,i}(R)dR}$$

We did not contain the meridional intensity data in the calculation for the reason mentioned before [3]. The *RMSI* is 0.133, lower than the value (0.351) before correction but the coincidence between the corrected intensities of a hexagonal-filament array model and those of a single filament model is not enough.

We carried out the simulation of the orientation of heads of crossbridges around the filament axis using the corrected layer-line intensities from a hexagonal-filament array model in order to make sure whether the optimum azimuthal orientation of heads obtained by this simulation is consistent with the orientation of heads of a single filament model. The result of the simulation showed that the azimuthal orientations of heads around a single filament are very similar to those of heads of a single filament model. Therefore we confirmed that this method is appropriate for correcting the partial sampling effects due to the hexagonal filament array on the observed layer lines, enabling us to obtain a single filament transform of myosin filaments. The modeling calculation of azimuthal orientations of two heads of myosin crossbridges around the filament axis in full-overlapped muscles by this method is shown in an accompanying report in this issue [4].

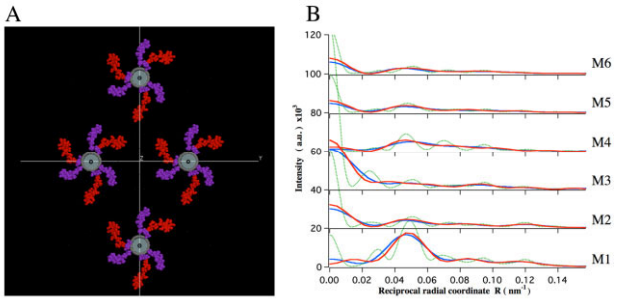

Figure 1. A, End-on view of a hexagonal-filament array model. Myosin two heads are denoted by red and purple spheres, respectively. B, Comparison of the layer-line intensities of a hexagonal-filament array model before (green dashed lines) and after correction (red lines) and those of a single filament model (blue lines).

References

[1] Oshima et al., PF Activity Rep. #23, 234. (2006).
[2] Namba et al., J. Mol. Biol. 138, 1-26 (1980).
[3] Oshima et al., J. Mol. Biol., 367, 275-301 (2007)
[4] Oshima et al., PF Activity Rep. #24 (2007) in press.

*waka@bpe.es.osaka-u.ac.jp