Biological Science

15A/2003G323

# Atomic Models of a Myosin Crossbridge Derived from Intensity Analysis of Myosin-based X-ray Meridional Reflections

Kanji OSHIMA, Yasunori TAKEZAWA, Yasunobu SUGIMOTO, and Katsuzo WAKABAYASHI*
Division of Biophysical Engineering, School of Engineering Science, Osaka University,
Toyonaka, Osaka 560-8531, Japan

## Introduction

The modeling analysis of the myosin-based meridional reflections in the X-ray diffraction patterns of live frog skeletal muscles at the full-overlap length of actin and myosin filaments in the relaxed and contracting states was reported in the previous report [1,2]. The derived density maps of the crossbridges projected onto the fiber axis had asymmetric profiles and became sharper in the contracting state than that in the relaxed state. On this basis, we progressed the atomic models of myosin crossbridges to reproduce the density maps of crossbridges in the relaxed and contracting states by calculating the mass projection of pairs of the crystallographically-determined structure of a myosin sub-fragment 1 (S1).

## Modeling calculation

The atomic coordinates of the α-carbons in the polypeptide chain of myosin heads were used for the simulation. Total number of the α-carbon was 2144 and each α-carbon was translated so that the origin of a Cartesian coordinate system was placed at the α-carbon (Pro840), which was thought to be close to the joint of two myosin heads. The simulation started from the atomic structure of a two headed myosin obtained by energy minimization, reported by Offer et al. (1996). The z-axis was assumed to be the fiber axis, onto which the mass projection was calculated. The myosin heads were rotated around the x-, y-, z-axes by α, β, γ, respectively, which variable ranges were limited: $0 \leq \alpha \leq 90$, $0 \leq \beta \leq 90$, and $0 \leq \gamma \leq 360$. Thereafter, the mass projection onto the z-axis was calculated by summing the projected density of the α-carbon which is approximated with the Gaussian function with 4σ (0.4 nm). The calculated mass projection was plotted in a 0.1 nm unit and the variation of the rotation was 15º.

## Results and Discussion

The mass projection onto the z-axis was then compared with the previously determined ones [1,2]. The most probable atomic model was determined by searching the best fit of the calculated density map to that previously reported [1,2]. The results of this simulation are shown in Fig.1, 2. The atomic structure in the regular region in the relaxed state was slightly different from that in the contracting state, although the mass projections were very similar. Each myosin head in the pair had a distinctly different axial orientation in the perturbed region both in the relaxed and contracting states as expected previously [1,2]. But the orientation of a myosin head around the fiber axis couldn't be determined because the rotation of a head around the fiber axis unaltered the projected density. The intensity analysis of the myosin-based layer line is necessary to determine the orientation of each head around the fiber axis.

## References

[1] Oshima et al., PF Activity Rep #21 (2004)
[2] Oshima et al., Fibre. Dif. Rev. 13 (2005)

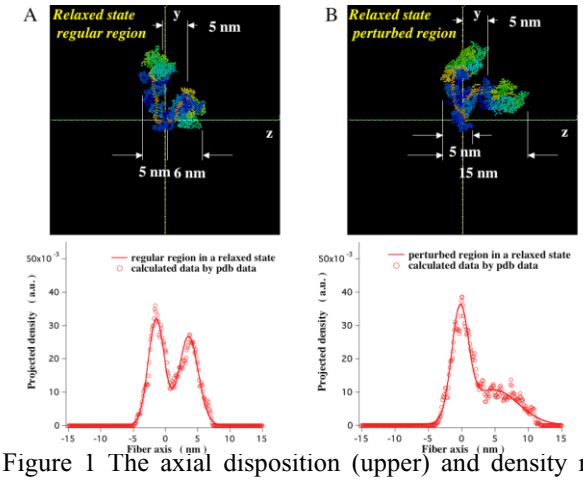


Figure 1 The axial disposition (upper) and density map (lower) of the two-headed myosin crossbridges. A; regular region, B; perturbed region.

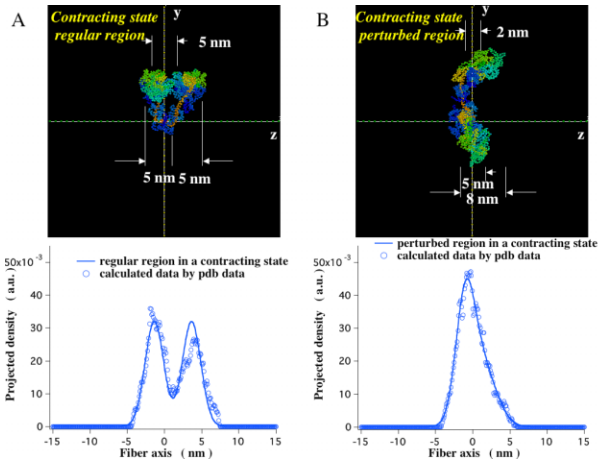


Figure 2 The axial disposition (upper) and density map (lower) of the two-headed myosin crossbridges. A; regular region, B; perturbed region.

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