Neutron scattering study on dynamics of hydration water around muscle contractile proteins

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In physiological conditions, proteins are surrounded by water molecules as solvent and fluctuating under their influence (in particular, hydration water molecules). It is now widely accepted that these thermal fluctuations, or the dynamics, of proteins are essential for their structural changes indispensable to their functions [1]. Since the dynamics of proteins is strongly coupled with that of hydration water [2], investigation of the dynamics of the hydration water is important for ultimate understanding of the protein functions.

In the previous study, we studied the density of the hydration shell around F-actin and myosin subfragment-1 (S1), which are proteins interacting with each other to produce force in muscle contraction, and found that the hydration shell around F-actin is denser than that around S1 [3]. This finding has raised the possibility that the dynamics of the hydration water around them could be also different. Characterizations of the dynamics of the hydration water around F-actin and S1 in addition to their structural properties are crucial for elucidating the role that the hydration water plays in muscle contraction.

Thus, in this study, we investigated the dynamics of the hydration water around F-actin and S1 by quasielastic neutron scattering (QENS). The QENS measurements were conducted on the solution samples of F-actin (150 mg/ml) and S1 (80 mg/ml) in H_2O and D_2O using the cold-neutron disk-chopper spectrometer AMATERAS in MLF/J-PARC, Japan. The spectra of hydration water were obtained by subtracting those of proteins and those of bulk water from the measured spectra of H_2O samples (the spectra of proteins were obtained by subtracting those of D_2O buffer from those of D_2O samples, while the spectra of H_2O buffer was used as those of bulk water) with appropriate scaling factors. The translational diffusion coefficients (D_T) and the residence time (τ_T) were evaluated from the dependence of the half-widths at half-maximum of the Lorentzian functions fit to the spectra on the momentum transfer.

In the current analysis, it was found that the D_T value of the hydration water around S1 was smaller than that of bulk water while the τ_T value was larger than that of bulk water, suggesting that S1 has typical hydration water, the mobility of which is less than that of bulk water. On the other hand, both the D_T and the τ_T values of the hydration water around F-actin were closer to those of bulk water, suggesting that the hydration water around F-actin has higher mobility than that around other proteins including S1. The results of a more detailed analysis will be given in the presentation.

References

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