Effect of temperature and pressure on protein dynamics studied by inelastic neutron scattering

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Protein structure fluctuates thermally, and the protein dynamics contributes to the stability and biological function. Protein dynamics has been described from the view point of the energy landscape. The structural fluctuation accompanies the volume fluctuation, indicating that protein dynamics should be characterized by the compressibility. Therefore, the effect of pressure as well as temperature on the protein energy landscape is essential for understanding the protein dynamics [1]. Inelastic neutron scattering (INS) is an effective method for studying the protein dynamics between picosecond and nanosecond time scales. So far the temperature dependence of protein dynamics in the powder state is well characterized, but the pressure effect on protein dynamics has not been studied well. Recently, the gas pressure system has introduced by O.Y. into the neutron spectrometer, AGNES. We performed INS experiment with AGNES, whose energy resolution is 120 μ eV, using Staphylococcal nuclease (SNase) of dehydrated samples at several sets of temperatures and pressures. Ar gas was used as pressure medium because of the relatively low background. Figures are the INS spectra at 160 K and 300 K under 1 atm and 900 atm. At 160 K pressure affects the low energy dynamics, whereas the vibrational spectrum with high frequency is not affected by high pressure. In the low energy region, the boson peak was observed, and the peak shifts to higher frequency at high pressure, suggesting potential hardening of protein collective modes. At 300 K and 1 atm, the quasi-elastic scattering appears aside the elastic peak, suggesting onset of the structural relaxation and/or diffusive dynamics. The quasi-elastic scattering significantly suppressed at high pressure and the boson peak was observed clearly, indicating that the protein conformation falls into a local minimum on the energy landscape at high pressure. Anharmonic motions were strongly suppressed by pressure. The anharmonic motions lost at high pressure should contribute to the biological function. Therefore, INS experiment along the axis of pressure as well as that of temperature is essential for analysis of the relationship between protein dynamics and function. Furthermore, the systematical studies of protein dynamics by the high-pressure INS experiment will open a new way to analyze the stability and function of the protein originated from the living organism in the deep sea (ex. Why is a deep-sea fish alive?) and give an important insight into the piezo-biology.

1) L. Meinhold et al. : "Proc.Natl.Acad.Sci. ", 104, 17261 (2007).

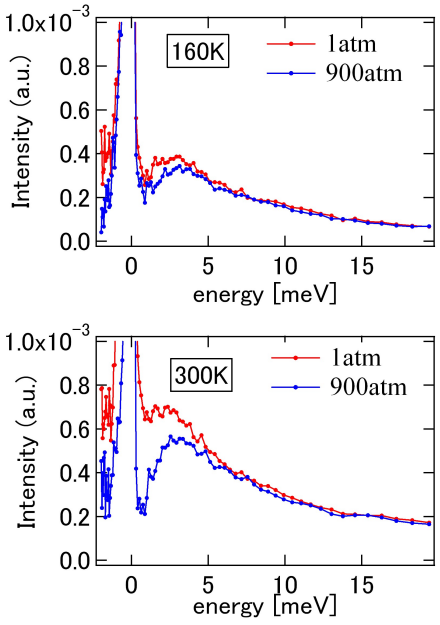

Fig. 1. INS spectra at 160 K and 300 K under 1 atm and 900 atm.