MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2009A0051 実験課題名 Title of experiment Effect of hydration on protein dynamics by TOF-elastic resolution spectroscopy 実験責任者名 Name of principal investigator Hiroshi Nakagawa 所属 Affiliation Japan Atomic Energy Agency	装置責任者 Name of responsible person Kenji Nakajima 装置名 Name of Instrument/（BL No.） BL−14 実施日 Date of Experiment 2005.12.15

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

Staphylococcal nuclease (SNase) D_2O-hydrated powder. The hydration level is 0.43 g D_2O/g protein.

2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）
Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

Inelastic neutron scattering measurements for the D_2O-hydrated SNase samples were successfully performed. Protein powder samples are put in the aluminum sample cell, and shielded with indium wire. Measurement temperatures are 100 K and 300K. Measurement energy resolution was changing by controlling the incident neutron energy (multi-Ei).

In this study the measurement time is quite limited because the allocation beam time is only one day. Furthermore, the sample change is possible only in day time, and it took 6-7 hours to change the sample. Therefore, we could not take a background measurement (empty cell).

The neutron spectrum at multi-Ei were shown in Fig.1. Table 1 shows the relation between flight time and Ei. In this study, we proposed the energy resolution scan experiment by incident neutron with multi-Ei, therefore, we successfully performed the Elastic Resolution Spectroscopy (ERS) method. We also measured the spectrum at lower energy mode, which is under analysis.

2. 実験方法及び結果（つづき） Experimental method and results (continued)

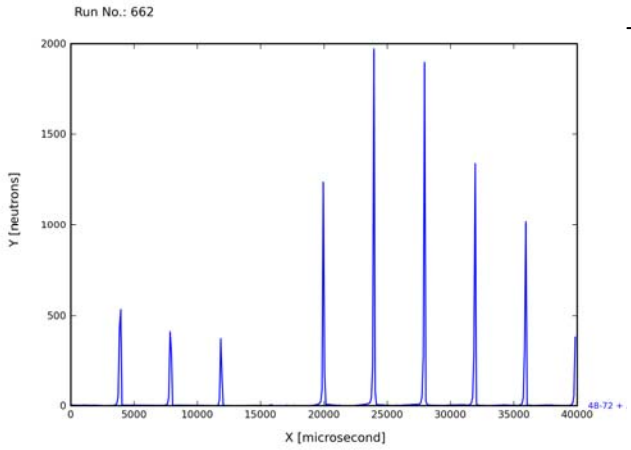


Figure 1

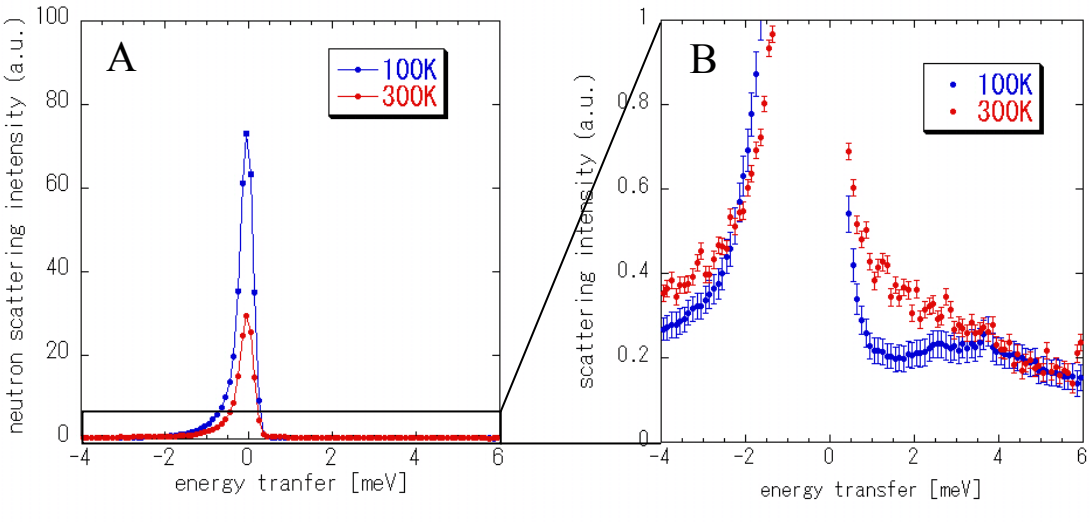
Neutron spectrum by multi-Ei

flight time [μs]	Ei [meV]
3910	3.134
7901	2.633
1890	2.244
19980	15.136
23967	10.519
27956	7.7314
31945	5.9211
35935	4.678
39923	3.7911

Table 1

Relation between flight time and Ei

Figure 2 shows the neutron inelastic scattering profiles of D_2O-hydrated SNase at 100 and 300K at incident neutron energy of 10.5 meV. The fig.2B shows that the strong elastic peak was observed at ω=0. The peak was stronger at 100K than at 300K. This is reasonable because the thermal motion of protein is active as the temperature increases. Accompanying the decrease of elastic peak, the quasi-elastic scattering was observed at 300K (fig.2B). This indicates the appearance of anharmonic motions. In fig. 2B, the broad peak around 3 – 4 meV was observed at 100K. This is boson peak of protein. These results are consistent with the previous our work. So far, it takes about one day to obtain the correspond data at a single Ei. Therefore, AMATERAS is effective to observe the protein dynamics with wide time scale using multi-Ei.



Neutron inelastic neutron scattering profiles of D_2O-hydrated SNase at 100 and 300K.
Incident neutron energy is 10.5 meV.