# MLF Experimental Report	提出日 Date of Report 2010 年 8 月 25 日
課題番号 Project No. 2010A0042 実験課題名 Title of experiment Sequence dependent DNA 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 2010.6.12-15, 22-25

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.

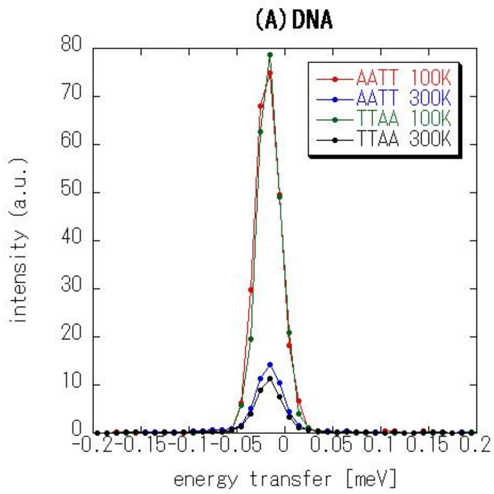
Two sequences of DNA, CGCGAATTCGCG and CGCGTTAACGCG. The sample form was powder.

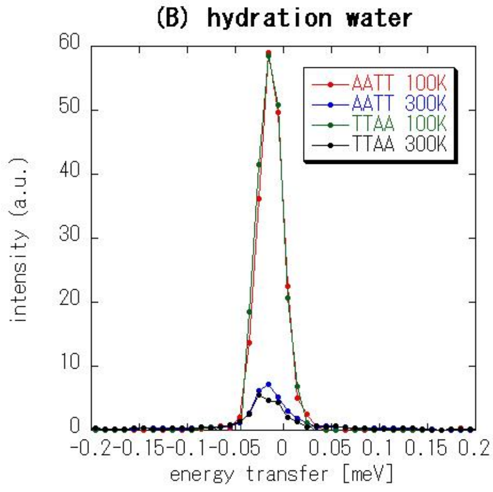
2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）
Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

Inelastic neutron scattering measurements for the D_2O and H_2O-hydrated DNA power samples were successfully performed. Protein powder samples are put in the aluminum sample cell, and shielded with indium wire. Measurement temperatures were from 100 K to 300K. Measurement energy resolution was changing by controlling the incident neutron energy (multi-Ei). We have proposed to examine the DNA sequence dependent dynamics of DNA molecules and its hydration water molecules in pico ~ nano second timescale by neutron scattering experiment. We have demonstrated that the sequence of DNA with CGCGTTAACGCG was softer than that with CGCGAATTCGCG by the molecular dynamics (MD) simulation. We measured the dynamics of DNA and its hydration water by neutron scattering experiment to verify the computational study.

We measured the neutron spectrum of DNA with the different energy resolutions by incident neutron with multi-Ei. We performed the experiments with high resolution mode. The incident neutron energies were 3.132, 1.685 and 1.050 meV. The DNA sample mass is about 200 mg. Figure A shows the neutron inelastic scattering profiles of D_2O-hydrated DNA for two sequences at 100 and 300K at incident neutron energy of 3.132 meV.

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





Figure

Neutron inelastic neutron scattering profiles of (A) DNA and (B) hydration water for AATT and TTAA sequences at 100 K and 300 K at incident neutron energy of 3.132 meV.

The figure A shows that the strong elastic peak was observed at ω=0. The peak was stronger at 100 K than at 300 K. This is reasonable because the thermal motion of DNA is active as the temperature increases. The elastic intensity of AATT is stronger than that of TTAA at 300 K. This suggests that AATT is less mobile than TTAA. This experimental result was qualitatively same as those with the different incident neutrons. This result agrees the prediction of MD simulation. Accompanying the decrease of elastic peak, the quasi-elastic scattering should be observed at 300K. We will analysis the quasi-elastic scattering.

Figure B shows the neutron inelastic scattering profiles of hydration water of DNA for two sequences at 100 K and 300 K at incident neutron energy of 3.132 meV. The scattering from hydration water was estimated by the subtraction of the scattering profile of D_2O-hydrated DNA from the H_2O-hydrated DNA. The elastic peak was weaker at 300 K than at 100 K by the thermal fluctuation of the hydration water. This suggests that the hydration water of TTAA is more mobile and/or diffusive than that of AATT. Furthermore, the sequence dependent dynamics of DNA corresponds to that of the DNA hydration water. This suggests that the hydration water dynamics activate the DNA fluctuation and water dynamics controls the DNA dynamics. The characterization of these dynamics will need the analysis of quasi-elastic scattering.

We successfully observed the dynamics of DNA and its hydration water by AMATERAS with multi-Ei. The results support the sequence dependent dynamics of DNA predicted by the molecular dynamics simulation. AMATERAS is effective to study dynamics of DNA and hydration water.