（ ※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。 ）

CROSS TOKAI **Experimental Report** J-PARC	承認日 Date of Approval 2014/10/1 承認者 Approver Kaoru Shibata 提出日 Date of Report 2014/8/19
課題番号 Project No. 2014A0108 実験課題名 Title of experiment Dynamical properties of soft confined water in lipid bilayers membrane 実験責任者名 Name of principal investigator Nobuaki Takahashi 所属 Affiliation Kyoto University	装置責任者 Name of Instrument scientist Kaoru Shibata 装置名 Name of Instrument/（BL No.） DNA / BL02 実施日 Date of Experiment 2014/05/21 21:00 - 2014/05/26 21:00

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.

d_{67}DMPC $15H_2O$ ($C_{36}D_{67}H_5NO_8P-15H_2O$)

d_{54}DMPC $15D_2O$ ($C_{36}D_{54}H_{18}NO_8P-15D_2O$)

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.

Dynamical behavior of confined water molecules has been studied intensively so far. The results indicated that the water dynamics is strongly influenced by the effect of confined walls. Most of these studies have been performed for water molecules within hard matter matrix. However, behaviors of water molecules within soft matter (soft-confined water) should also be interesting from the viewpoints of biological functions. The dynamics of the DMPC / water system has been focused in this study. In order to understand whole dynamics of the system, the partially deutrated samples to distinguish the dynamics of the each part (alkyl chain, water and hydrophilic group) have been used. In this proposal, the temperature dependence of the d_{67}DMPC•$15H_2O$ and d_{54}DMPC•$15D_2O$ for observing dynamics of the water and hydrophilic part, respectively, was investigated. The elastic scan of d_{67}DMPC•$15H_2O$ was performed between 50 and 330 K with 1 $Kmin^{-1}$. The QENS measurements of d_{67}DMPC•$15H_2O$ and d_{54}DMPC•$15D_2O$ were performed at 317, 306, 296, 286, 276 and 266 K with 3.5 μeV energy resolution. The each counting time was around 5 h including temperature control.

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

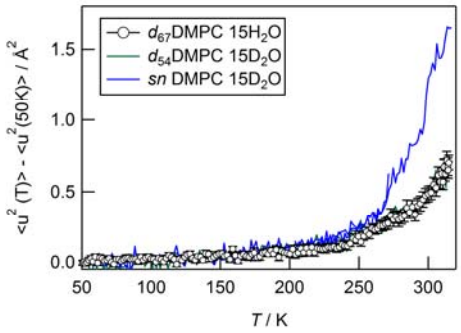

Fig. 1. Mean square displacements of DMPC • 15 H_2O systems having different deutaration parts.

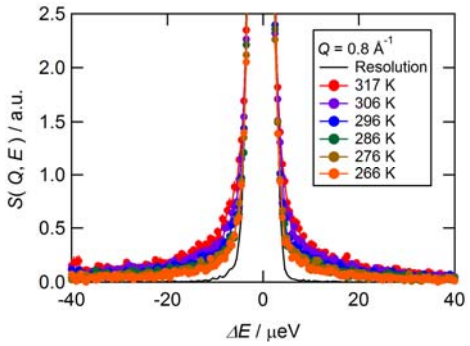

Fig. 2. QENS profiles of d_{67}DMPC•15H_2O at Q = 0.8 Å^{-1} and different temperatures.

Fig. 1 shows mean square displacements (<u^2>) of DMPC • 15 H_2O systems. The <u^2> of d_{67}DMPC•15H_2O was the same as that of d_{54}DMPC•15D_2O and showed no jumps around 273 K. This result indicated that the adsorbed water was bound and cooperated with the hydrophilic group. The QENS profiles of d_{67}DMPC•15H_2O were shown in Fig. 2. The QENS broadening was observed within the measured temperature range.

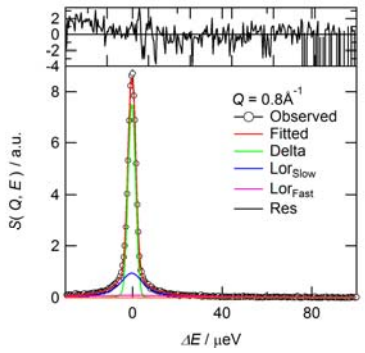

Fig. 3. QENS profile of d_{67}DMPC•15H_2O and fitted results at 0.8 Å^{-1} and 317 K.

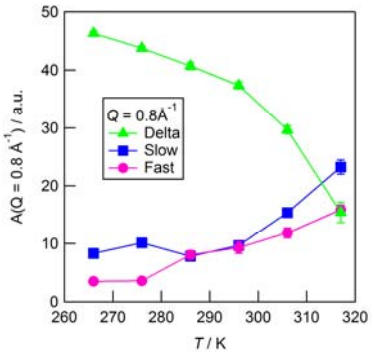

Fig. 4. Temperature dependence of each component of d_{67}DMPC•15H_2O at 0.8 Å^{-1} obtained by the profile fitting.

The QENS profile was well fitted by sum of a delta function, two Lorentz function and constant background convoluted with the resolution function. The obtained fitting result of d_{67}DMPC•15H_2O was shown in Fig. 3. The intensity of the each component obtained by the profile fitting plotted to the temperature in Fig. 4. The phase transition called as “main transition” occurred around 297 K (Fig.1) and mainly related to the conformational change of the alkyl chain in the hydrophobic part. However the dependence of the both Lorentz function corresponding to the water motion is also changed around 297 K. This result indicated that the adsorbed water motion was affected by the dynamics of the hydrophobic part. Further analysis is in progress.