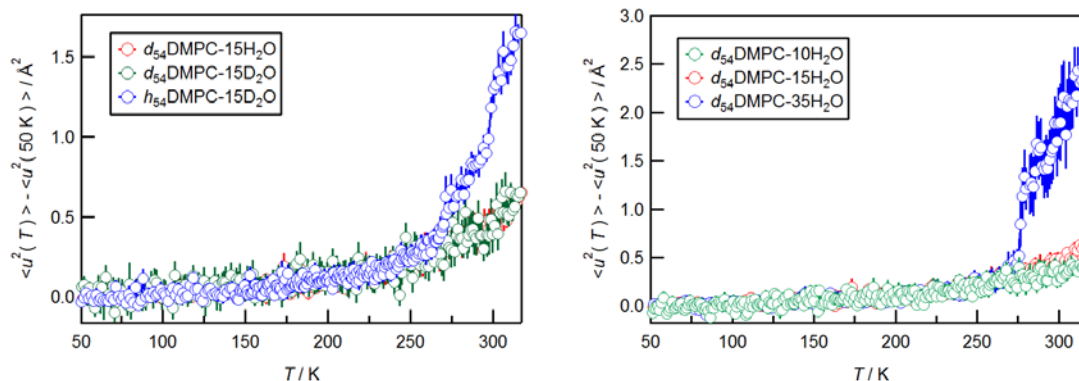
	承認日 Date of Approval 2013.9.18 承認者 Approver Kaoru Shibata 提出日 Date of Report 2013.8.30
実験課題番号 Project No. 2012P0402 実験課題名 Title of experiment Dynamics of water molecules in soft matters (A: Lipid bilayers membrane, B: Hydro gels) 実験責任者名 Name of principal investigator Nobuaki Takahashi 所属 Affiliation J-Parc Center	装置責任者 Name of Instrument scientist Kaoru Shibata 装置名 Name of Instrument/(BL No.) DNA / BL02 利用期間 Dates of experiments 2012/12/17 ~ 2012/12/21 2013/01/20 ~ 2013/01/23

<p>1. 研究成果概要(試料の名称、組成、物理的・化学的性状を明記するとともに、実験方法、利用の結果得られた主なデータ、考察、結論、図表等を記述してください。</p> <p>Outline of experimental results (experimental method and results should be reported including sample information such as composition, physical and/or chemical characteristics.</p> <p>Water is one of major materials in our life; ex. 70% surface of the earth is covered by water or 70 wt % is water in a human body. On the other hand, Water is strange liquid from a view point of science; ex. the density exhibits maximum at 237 K or the isothermal compressibility is diverse around 233 K. Therefore many researchers are studied for the anomalies by various approaches. Neutron scattering is one of the most powerful tools for studies on water because of the large scattering cross section of hydrogen. Water in confined space which exhibit large super-cooling below homogenous nucleation temperature are studied by quasi-elastic neutron scattering (QENS). The dynamical transition from non-Arrhenius type to Arrhenius type of the confined water in meso-porous materials is reported using QENS and is related to second critical point of water.</p> <p>On the other hand, phospholipids which is one of the main components in biomembranes form bilayer structure in the aqueous solutions where the hydrophilic and hydrophilic groups directed to the outside and the inside, respectively. 1,2-dimyristoyl-sn-glycero- 3-phosphocholine (DMPC) forms lamella structure consisting of 2 nm bilayer of the DMPC and a few nm of water layer which depends on the water concentration. Hishida et.al. reported that the hydration number to one DMPC is 28 by THz spectroscopy and that the water forms hydration layer with four or five layers(Hishida and Tanaka, PRL 106, 158102 (2011)). The hydration number is decided by subtraction between the DMPC hydrate spectra and that of bulk water. By contrast, QENS is possible directly to measure the dynamics of the hydrated water and bulk water. In order to understand whole dynamics of water in DMPC hydrate, QENS measurements were performed in this project.</p> <p>The DMPC hydrates having different water contents were prepared by the simple mixing. Deuterated water and d_{54}DMPC having deuterated long alkyl chains are used to distinguish dynamics of water and alkyl chains. The samples were wrapped with aluminum foils and loaded into aluminum cells. The</p>
--

1. 研究成果概要(つづき) Outline of experimental results (continued).



QENS measurements and elastic scans were performed using BL02 DNA spectrometer.

The left figure shows mean square displacements ($\langle u^2 \rangle$) of DMPC-15H₂O hydrates system having different contrast. The $\langle u^2 \rangle$ of h_{54} DMPC-15D₂O corresponding to the scattering from the alkyl chains exhibited jumps around 270K and 300 K. These are due to the phase transition among the gel (L_{β}'), ripple (P_{β}') and fluid phases (L_{α}') from lower temperature side, respectively. On the other hand, the $\langle u^2 \rangle$ of d_{54} DMPC-15H₂O and d_{54} DMPC-15D₂O corresponding to the scattering from the water and the hydrophilic group, respectively, shows slight deviation from linear relationship around 225 K. Additionally, The $\langle u^2 \rangle$ of d_{54} DMPC-15H₂O showed no jumps at 273.15 K due to melt of bulk water. These results indicate that all water in the DMPC-15H₂O is interacted with the hydrophilic group and the dynamics of the adsorbed water is different from that of bulk water.

The right figure shows $\langle u^2 \rangle$ of d_{54} DMPC- n H₂O ($n = 10, 15, 35$). In case of $n = 35$, the $\langle u^2 \rangle$ exhibited a jump around 273 K. Meanwhile, no jumps observed in $n = 10$ and 15. These results indicate that free water like bulk water exists in d_{54} DMPC-35H₂O. The $\langle u^2 \rangle$ at 320 K are different between $n = 15$ and 10. This result indicates that the dynamics of the adsorbed water on the hydrophilic group depend on the hydration number. Further analysis of QENS profiles is in progress.

必要に応じて、A4 サイズの用紙に続きを記入して下さい。

Please use A4-size papers for further reporting, if necessary.