（ ※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。）

MLF Experimental Report

課題番号 Project No. 2014A0326	提出日 Date of Report 2014/07/14
実験課題名 Neutron Brillouin scattering of liquid methanol	装置責任者 Name of responsible person Shinichi Ito
実験責任者名 Koji Yoshida	装置名 Name of Instrument/（BL No.） HRC(BL12)
所属 Affiliation Fukuoka university	実施日 Date of Experiment 2014/05/23～2014/05/27

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.

Liquid metnanol-d4（CD_3OD）

Liquid methanol-d（CH_3OD）

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.

Liquid methanol was sealed into a rectangle cell made of aluminum. Inner dimensions of the cell were 30 x 30 x 9.5 mm^3. Indium wire was used for seal. The cell was stored in the vacuum chamber of the HRC spectrometer. The measurement was performed at room temperature. Phononic excitations in a liquid methanol were measured with E_i = 102 meV and ΔE= 2.0 meV. The background-subtracted spectra showed excitation peaks and a resolution-limited elastic peak. The excitation peaks were fitted with a damped harmonic oscillator (DHO) function convoluted with the resolution width multiplied by a temperature factor.

$$S(Q,\omega)=\left[\frac{\hbar\omega/k_BT}{1-\exp(-\hbar\omega/k_BT)}\right]\frac{A_0}{\pi}\frac{\Gamma_0}{\Gamma_0^2+\omega^2}+\left[\frac{1}{1-\exp(-\hbar\omega/k_BT)}\right]\times\frac{A(Q)}{\pi}\frac{4\omega\Gamma(Q)\sqrt{\Omega(Q)^2-\Gamma(Q)^2}}{(\omega^2-\Omega(Q)^2)^2+4\omega^2\Gamma(Q)^2}$$

where A_0 and Γ_0 are the intensity and width of a central peak, respectively. $A(Q)$ and Γ(Q) are the intensity and width (damping factor) of the inelastic peaks, respectively, at positions $\pm\Omega(Q)$ of an DHO peak due to inelastic scattering.

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

Fig. 1 shows a typical spectrum of methanol-d4 at room temperature. Solid line indicates the fitting result by the DHO model. The high frequency sound velocity of liquid methanol-d4 is obtained from the dispersion relation between the inelastic excitation peak $\Omega(Q)$ and the momentum transfer Q. Since the adiabatic sound velocity of liquid methanol is 1094 ms^{-1}, the positive dispersion of liquid methanol-d4 is about 50 %. This is similar value obtained from inelastic X-ray scattering of protonated methanol [1].

Elastic peak of methanol-d was higher than that of methanol-d4 due to the incoherent scattering of hydrogen atoms of methanol. Since DHO peaks were relatively small, the fitting process was difficult. The inelastic excitation peak $\Omega(Q)$ was ~2.4 meV, independent of Q. To assign this mode, MD simulation of liquid methanol will be performed.

[1] K. Yoshida, N. Yamamoto, S. Hosokawa, A.Q.R. Baron, T. Yamaguchi, Chem. Phys. Lett. 440 (2007) 210–214.

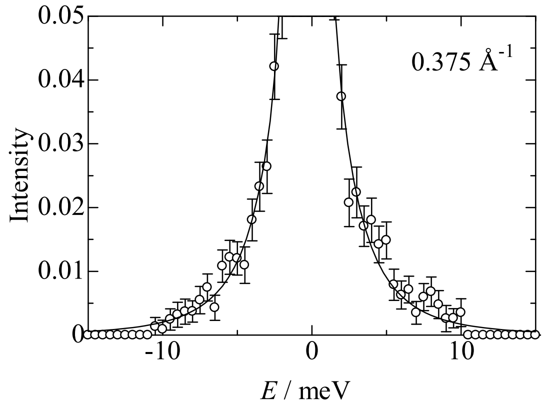

Fig.1. The neutron Brillouin spectrum of liquid methanol-d4, $S(Q, E)$ at Q = 0.375 Å^{-1} at room temperature. The solid line indicates the fitting result by the DHO model

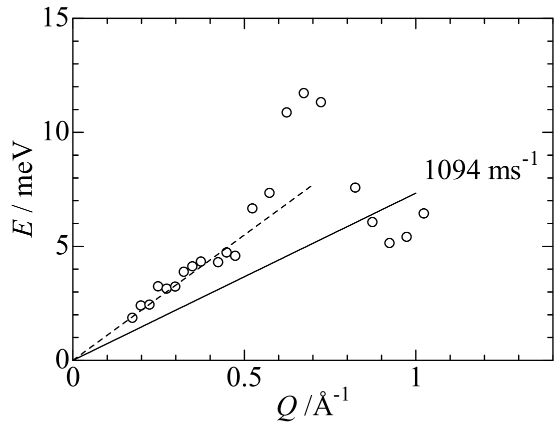

Fig.2. Dispersion relation between the inelastic excitation peak $\Omega(Q)$ and the momentum transfer Q for liquid methanol-d4 at room temperature. The dashed line show the least-square fit in a low Q-region. The high-frequency sound velocity was obtained from the slope of the fit. The solid line shows the adiabatic sound velocity of liquid methanol.