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 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2013B0229 実験課題名 Title of experiment Study on diffusion dynamics varied with intra- and intermolecular structures in benzene-like liquids by mode distribution analysis 実験責任者名 Name of principal investigator Kikuchi Tatsuya 所属 Affiliation J-PARC Center	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 2014/4/2 - 2014/4/7

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. xylitol $C_5H_{12}O_5$ D-sorbitol $C_6H_{14}O_6$ n-pentane C_5H_{12} m-hexane C_6H_{14}
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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. <p>Four samples were loaded into the double cylindrical Al can and sealed with indium gasket respectively beforehand outside MLF. We used the standard cryostat of AMATERAS and top-loading cryostat of BL-01, SIKI for the measurements. Each sample was measured at several temperatures in 180 - 560 K. The measurements mainly were carried out under the settings of low energy and high resolution with multi E_i set of 42.1, 7.7, 3.1 and 1.7 meV. Data acquisition times were 4 - 5 h at the operation with 300 kW proton-beam power of J-PARC, respectively. Figure 1 shows the examples of $S(Q, \omega)$'s by the measurements. The statistics precision was an acceptable level for analysis of quasielastic neutron scattering (QENS)</p> <p>We analyzed the data by mode distribution analysis (MDA) as wrote for the proposal of this experiment. In this method, $S(Q, \omega)$ can be described,</p> $S(Q, \omega) = A(Q)\delta(\omega) + \int B(Q, \Gamma) \frac{1}{\pi} \left(\frac{\Gamma}{\omega^2 + \Gamma^2} \right) d\Gamma.$
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2. 実験方法及び結果(つづき) Experimental method and results (continued)

$B(Q, \Gamma)$ is an intensity distribution for HWHM of Lorentzian. This function can show the number of modes and distributions of the relaxation times in the modes and we call it as mode distribution function (MDF). In this new approach, we can obtain $B(Q, \Gamma)$ by using the maximum entropy method (MEM). Figure 2 shows the examples of obtained $B(Q, \Gamma)$'s by this method. From these results, we found that three very broad modes unlike simple molecular liquid like benzene which we experimented on last time.

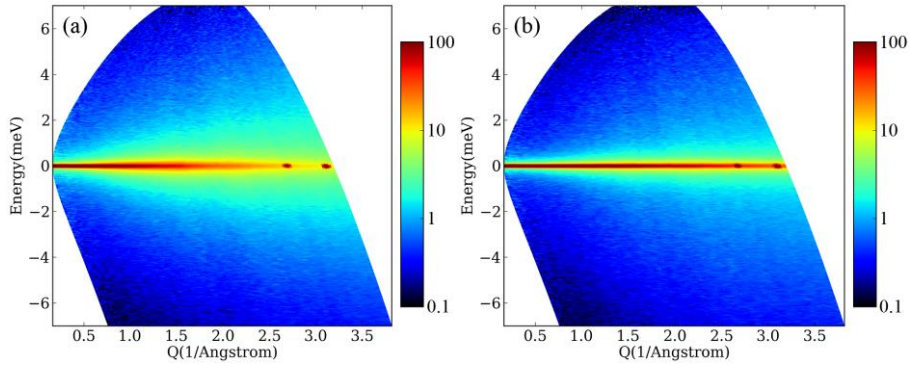


Fig. 1 $S(Q, E)$ maps of liquids at $E_i = 7.7$ meV. (a) n-pentane at 143 K. (b) xylitol at 403 K.

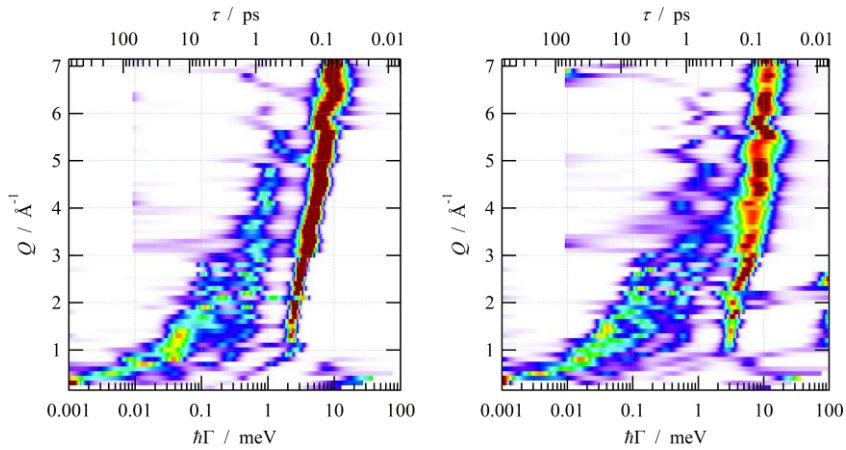


Fig. 2 $B(Q, \Gamma)$ maps of (a) n-pentane at 143 K and (b) xylitol at 403 K.