MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2014B0215 実験課題名 Title of experiment Elucidation of intermediate mode on dynamics of water by mode distribution analysis 実験責任者名 Name of principal investigator Kikuchi Tatsuya 所属 Affiliation J-PARC Center, JAEA	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 2015/4/23 - 2015/4/25 2016/4/16 - 2016/4/18 2016/5/9 - 2016/5/11

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.

Water H_2O

Deuterated Water D_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.

We prepared bulk H_2O and D_2O samples. In addition, we prepared H2O samples for super cooling in about a hundred capillaries. All water samples were loaded into the double cylindrical Al can and sealed with indium gasket respectively beforehand outside MLF. We used the top-loading cryostat with the bulk samples and the bottom-loading cryostat with the capillary sample. Each sample was measured at several temperatures within 254 - 353 K. The measurements were carried out under the settings of low energy and high resolution with multi E_i set of 1.7, 3.1, 7.7 and 42 meV. Data acquisition times were 4 – 12 h at the operation with 200 kW proton-beam power of J-PARC, respectively.

We analyzed the $S(Q,\omega)$ by mode distribution analysis (MDA) as wrote for the proposal of this experiment. In this method, $S(Q,\omega)$ can be described,

$$S(Q,\omega) = A(Q)\delta(\omega) + \int B(Q,\Gamma)\frac{1}{\pi}\left(\frac{\Gamma}{\omega^2+\Gamma^2}\right)d\Gamma.$$

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 Loretzian. 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). Figure shows the obtained $B(Q,\Gamma)$ maps of H_2O at several temperatures. From our previous study, we have founded that H_2O liquid have three diffusive modes. We that concluded that the slowest mode is translational diffusion of water molecules and the fastest mode is local fluctuation mode. In addition, The intermediate mode is thought of as local diffusion mode like a rotational of molecules. From this results, we found that the intermediate mode has low temperature dependency of the relaxation time and high temperature dependency of its intensity. We will elucidate the origin of the intermediate mode to continue the analysis of the results.

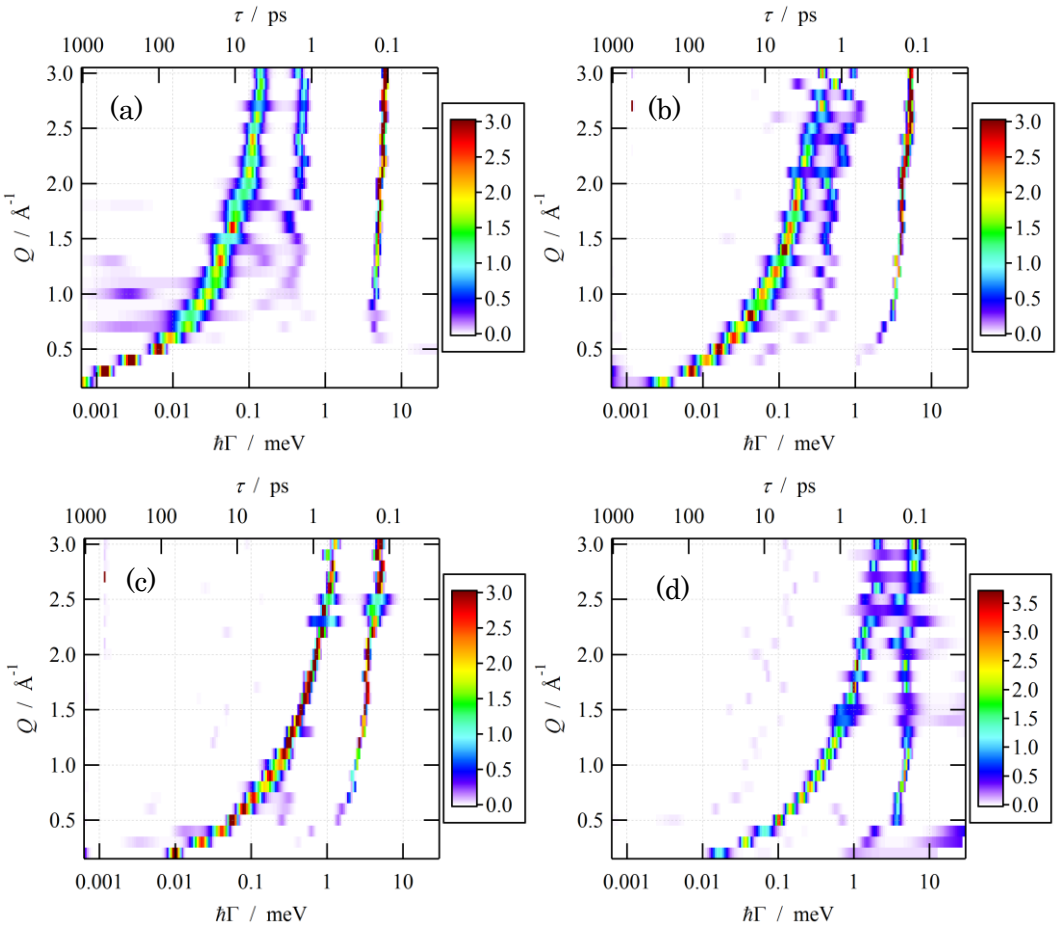

Fig. $B(Q,\Gamma)$ maps of H_2O at (a) 254K, (b) 273 K, (c) 318 K and (d) 354 K.