MLF Experimental Report	提出日 Date of Report 8/26/2016
課題番号 Project No. 2014B0262 実験課題名 Title of experiment QENS Study of the Dynamics of the prepeak in… 実験責任者名 Name of principal investigator Antonio Faraone 所属 Affiliation NIST Center for Neutron Research	装置責任者 Name of responsible person 装置名 Name of Instrument/（BL No.） AMATERAS/BL14 実施日 Date of Experiment

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.

Isopropanol (Liquid)
C3H7OH
C3D7OD
C3H7OD
C3D7OH

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.

The experiment 2014B0262 was scheduled to be performed starting on February 22nd 2015 until March 4 2015. Unfortunately, during that period some issues where experienced with the neutron source. For this reason, the experiment could not be performed as scheduled. However, thanks to the help of the Amateras instrument scientist all the planned measurements were eventually performed. Data were collected on four samples of the mono hydroxyl alcohol isopropanol differing for their deuteration: namely isopropanol-d8, isopropanol-d7, isopropanol-OD, and isopropanol-h8. Measurements were performed for all these samples in the temperature range from 260 K to 180 K with 20 K steps. An additional measurement at 20 K was used as instrumental resolution function. Multiple incoming energy, E_i, spectra were collected at the same time for E_i=7.7 meV, 3.1 meV, and 1.7 meV.

The quality of the obtained data is very good. In Fig. 1a, an example of the data collected on the perdeuterated sample at 260 K with Ei=3.1 meV is shown. The First Sharp Diffraction Peak can be clearly identified at Q≈1.5 $Å^{-1}$, together with the prepeak at Q≈0.8 $Å^{-1}$. As a comparison, in Fig. 1b,

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

the corresponding data for isopropanol-d7 are shown. The FSDP is still visible, although not as clearly, whereas the prepeak cannot be identified visually. In this case the incoherent scattering is a stronger component of the spectra and the structural features are less visible.

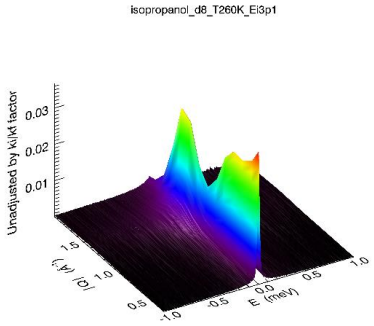

Fig. 1a

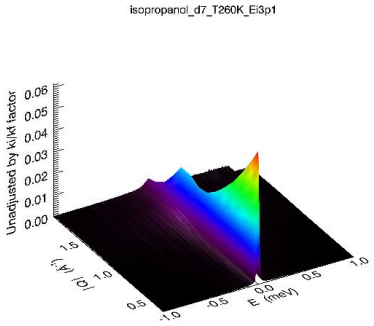

Fig. 1b

The data are being analyzed using different methods. In a first analysis, the data have been Fourier transformed to the time domain to obtain the normalized intermediate scattering functions I(Q,t)/I(Q,0) and corresponding data for different Ei have been concatenated to obtain one spectra. The obtained data at the same Q for different temperatures have been fit using a stretched exponential: $I(Q,t)/I(Q,0)=A\ Exp\ [-(t/\tau)^{\beta}]$. Where A and β are assumed to be temperature independent. Fig. 2 exemplifies the results of such analysis.

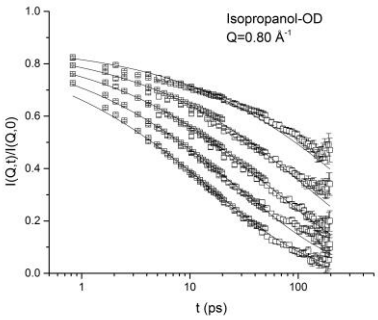

Fig. 2

In a second method of analysis a global fitting of data in the energy domain at the same Q value but of different Ei was performed. The fitting function was in this case:

$$S(Q,E) = A\ FT\left\{I_1 \exp\left(-\frac{t}{\tau_1}\right) + (1-I_1)\exp\left[-\left(\frac{t}{\tau_2}\right)^{\beta}\right]\right\} + BKG$$

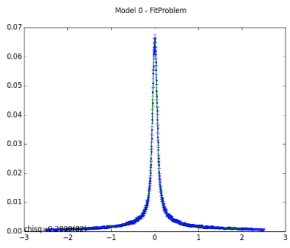

Fig. 3a

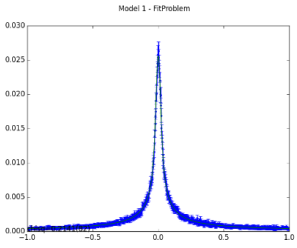

Fig. 3b

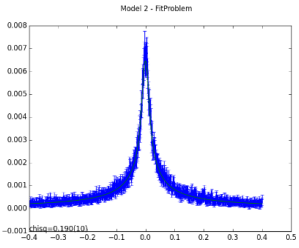

Fig. 3c

Fig. 3 shows an example of the obtained fits. The obtained fitting parameters are currently being interpreted to obtain a picture of the molecular dynamics of the H-bonded structures in isopropanol.