


(※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。)

 <b>MLF Experimental Report</b>	提出日 Date of Report
課題番号 Project No. 2012A0046 実験課題名 Title of experiment QENS Study of the Coherent Dynamics of H-bonded Clustering Alcohols 実験責任者名 Name of principal investigator A. Faraone 所属 Affiliation NIST Center for Neutron Research and University of Maryland	装置責任者 Name of responsible person K. Nakajima, T. Kikuchi 装置名 Name of Instrument/(BL No.) BL14 実施日 Date of Experiment 2012/10/20 21 : 00 - 2012/10/27 13 : 00

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.
2-Propanol, C <sub>3</sub> D <sub>7</sub> OD, liquid

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 collective dynamics of isopropanol was investigated in the liquid and supercooled state through QENS measurements of perdeuterated isopropanol.

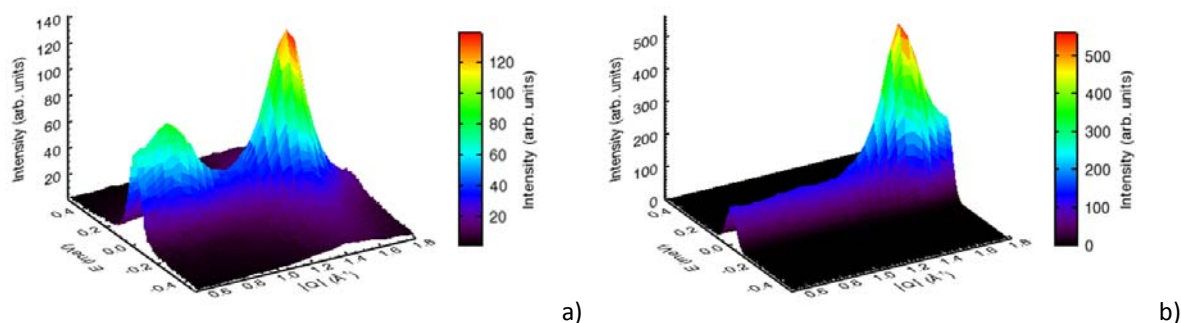


Fig. 1 Examples of data collected in the liquid state (a T=280 K) and supercooled state (b T=110 K).

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

The data have been analyzed in the time domain after Fourier transform of the spectra to take advantage of the multi-resolution measurements. A stretched exponential function was used to fit the data. The amplitude and stretching exponent was allowed to change with  $Q$  but not with temperature (see fig. 2):

$$\frac{I(Q,t)}{I(Q,0)} = A(Q) \exp \left[ - \left( \frac{t}{\tau(Q,T)} \right)^{\beta(Q)} \right]$$

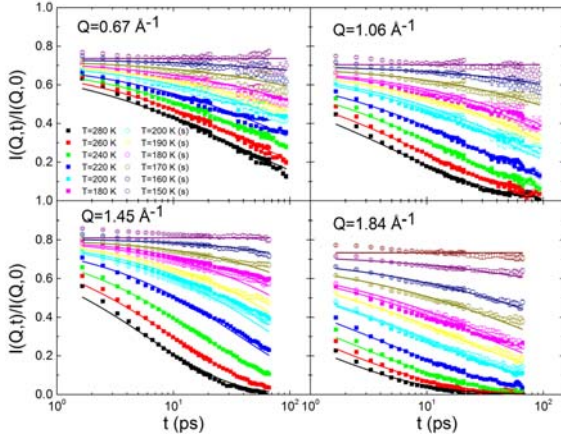


Fig. 2 Example of obtained data and fitting results.

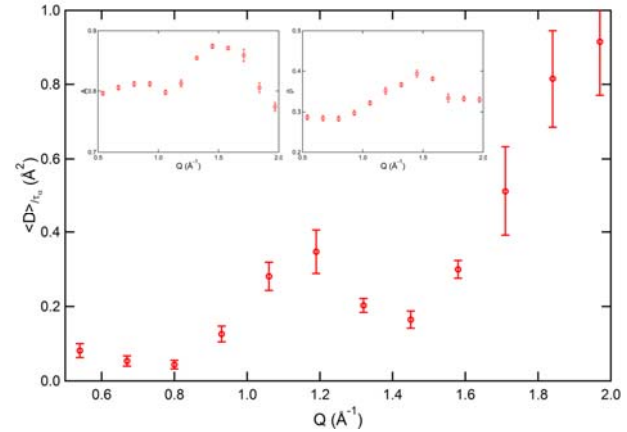


Fig. 3 Q dependence of the fit results (the relaxation time is normalized to the  $\alpha$ -relaxation time scale)

The obtained results indicate a significant slowing down of the dynamics in correspondence of the prepeak (see fig. 3).

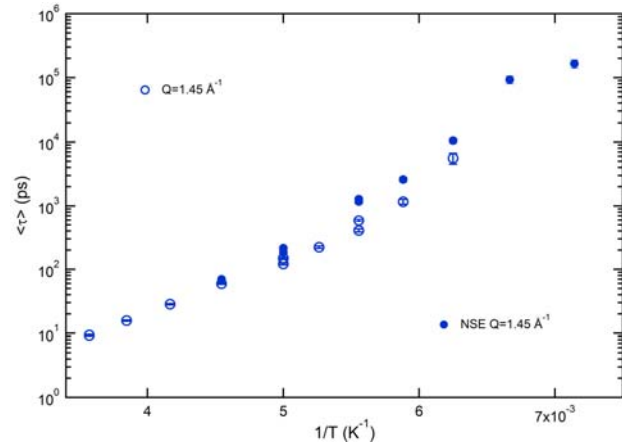
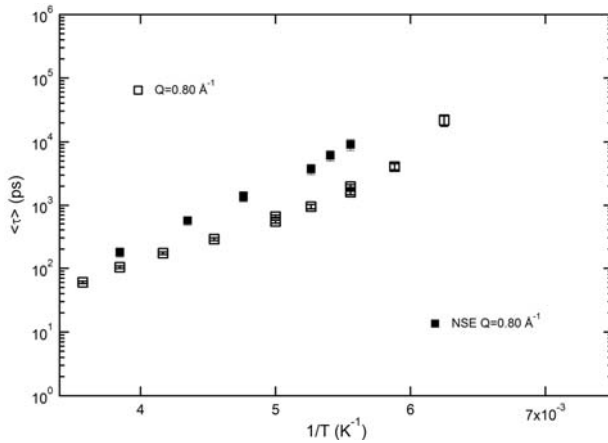


Fig. 4 The obtained relaxation times compared with the results measured with NSE.

The obtained relaxation times agree were compared with the results from the Neutron Spin Echo (NSE) spectrometer at NIST. The agreement is very good at the first sharp diffraction peak. These data can be analyzed in the liquid and supercooled state in terms of a Vogel Fulcher Tamman equation. Some inconsistency between the NSE and Amateras data was observed at the prepeak, which is probably associated with the contribution from incoherent scattering.

The data collected are probably going to result in an interesting publication once the effect of incoherent scattering is clarified.