
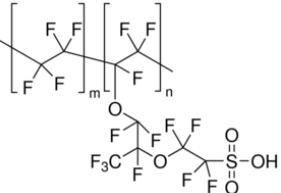


(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

	承認日 Date of Approval 2015/7/8 承認者 Approver Kaoru Shibata 提出日 Date of Report 2015/7/8
課題番号 Project No. 2014B0181 実験課題名 Title of experiment Selective solvation of Nafion in 1-Propanol/Water solution 実験責任者名 Name of principal investigator Makoto Yamaguchi 所属 Affiliation Fuel Cell Cutting-edge Research Center	装置責任者 Name of Instrument scientist Kaoru Shibata 装置名 Name of Instrument/(BL No.) BL-02 実施日 Date of Experiment April 24-26, 2015

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.
<p>Nafion (2.2wt%) dispersed in 1-C₃H₇OD/D₂O (23/77 v/v). The solution looks colorless and transparent, indicating Nafion particles are uniformly dispersed. 1-C₃H₇OD/D₂O (23/77 v/v) solution without Nafion was also prepared for comparison.</p>  <p style="text-align: center;">Chemical structure of Nafion</p>

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>Experimental method</p> <p>Measurement cells were made of two cylindrical quartz cells (thickness 0.5mm) with different diameter (13.4 and 14mm). The sample solution was carefully poured into the small gap between the two cells to avoid bubble formation. The quartz cell was placed in an aluminum cell for measurement.</p> <p>Sample measurements were performed at 300 and 285K. Incident energy of neutron was selected by the choppers and kinetic energies of the scattered neutrons were detected with the high-resolution mode. The energy range of the scattered neutrons was -400 to 600 μeV, which was covered by combinations of eleven accumulation steps performed by shifting 30 ~ 35 μeV the energy range. Energy resolution was 3.6 μeV. Total accumulation time for one sample was about 5.5 hours. Actually we prepared other two samples with different composition but found that Nafion was not uniformly dispersed in them. We had to work with only one Nafion sample and its solvent as another one and thus we tried to measure them at two different temperatures. A blank cell was also measured as the background data.</p>

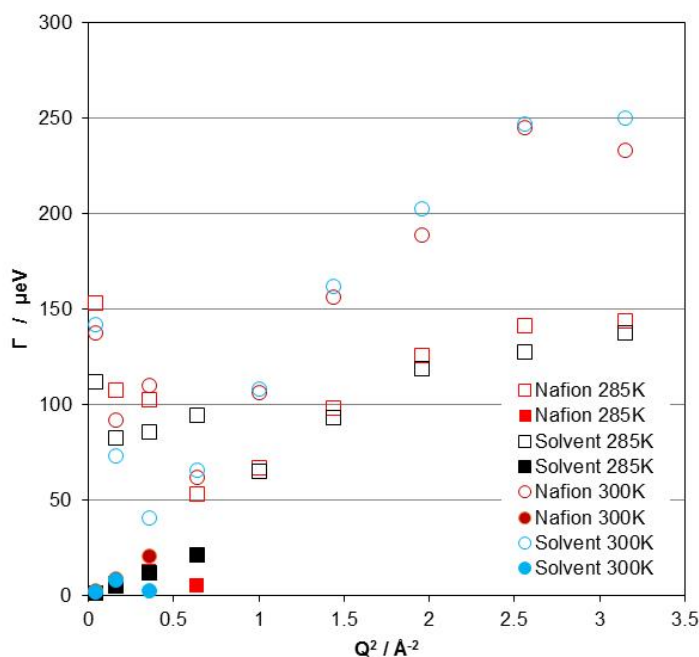
2. 実験方法及び結果(つづき) Experimental method and results (continued)

Results

The measured $S(Q,E)$ data were binned from $0.2 \sim 1.6 \pm 0.075 \text{ \AA}^{-1}$ in 0.2 \AA^{-1} steps and $1.725 \pm 0.05 \text{ \AA}^{-1}$. Thus obtained $S(E)$ data were analyzed by using 1D peak fitting of DAVE program (version 2.3). The measured $S(E)$ data were deconvoluted with the dataset of the blank cell ($\pm 20 \text{ \mu eV}$) and one ($Q \geq 1.0 \text{ \AA}^{-1}$) or two ($Q \leq 0.8 \text{ \AA}^{-1}$) Lorentzian curves and a linear background. χ^2 values of the fittings were $1.5 \sim 3.7$.

For data with $Q \geq 1.0 \text{ \AA}^{-1}$ gamma values of the Lorentzians plotted against Q^2 show steady increase at up to ~ 2.5 and then become constant which are typical for jump diffusion model, regardless of the presence of Nafion in the samples. The gamma values at 300K are much larger than those at 285K as expected. However, while the Nafion solution showed slightly larger gamma values than those of the solvent at 285K, this trend is opposite at 300K. Diffusion coefficients and mean residence times were estimated from these data based on the jump diffusion model and they are summarized in the table. The diffusion coefficients were about half of the measured value of $\sim 6.0 \times 10^{-10}$ in 1-propanol/water mixture with or without salt (Hawlicka and Grabowski, J. Phys. Chem. 96, 1554(1992)).

At $Q \leq 0.8 \text{ \AA}^{-1}$ two Lorentzians were necessary to fit each $S(E)$ profile. One of the two gamma values is very small and decreases towards smaller Q , while another is about ten times larger and increases towards smaller Q . At this moment we have not given any interpretation for those two gamma values yet.



	$D / \text{m}^2 \text{ s}^{-1}$	τ_0 / s
Nafion 285K	2.0×10^{-10}	1.0×10^{-11}
Solvent 285K	2.0×10^{-10}	1.2×10^{-11}
Nafion 300K	3.1×10^{-10}	5.5×10^{-12}
Solvent 300K	3.1×10^{-10}	4.5×10^{-12}