


実験報告書様式(一般利用課題・成果公開利用)

(※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。)

 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2016A0153 実験課題名 Title of experiment Molecular structure of ethanol/water surface 実験責任者名 Name of principal investigator: Dr. Chi M. Phan 所属 Affiliation Curtin University, Australia	装置責任者 Name of responsible person Dr. Norifumi L. Yamada 装置名 Name of Instrument/(BL No.) BL16 実施日 Date of Experiment: 26/01/2017 to 29/01/2017

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.
D2O, H2O, deuterated methanol: in liquid form NaCl: in solid form

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.
(This area is currently blank for the user to provide experimental details.)

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

The role of molecular arrangement of surface tension has been proposed in the literature more than 100 years ago. Yet, the exact nature of the arrangement remains elusive. Recently, our simulations have demonstrated that the molecular arrangement can be directly related to surface energy of ethanol/water mixture. It revises the Langmuir's theory, in 1925. Yet, the molecular arrangement is complicated and difficult to assess. While the surface tension can be measured routinely, the data alone is insufficient to deduce the molecular arrangement. In this study, we aim to explore the molecular nature of ethanol/water interface by combining neutron reflectometry, surface tension and simulations. To achieve this, surface excess of d-ethanol at the interface was measured directly by neutron reflectometry using SOFIA reflectometer. The reflectivity profiles were fitted using the monolayer model and MOTOFIT software to produce the SLD of the layers, their distribution and the surface excess. The data is then combined with surface tension and simulation to deduce molecular arrangement. More specific, the arrangement of methyl group on water surface layer will be described. The novel results will provide fundamental insights into the first molecular layer of alcohol solutions, which are employed widely in many activities.

Experimental details: 10 solutions of d-ethanol and D2O/H2O were prepared and measured, both surface tension and neutron reflectometry. The data is still being analysed and will be compared with modeling. Some samples of reflectometry are included below.

