Dynamics of ice Ih films upon methanol adsorption : quasielastic neutron scattering experiments and molecular dynamics simulations

Stéphanie Lucas, Daniel Ferry, Benjamin Demirdjian, Jean Suzanne, Sylvain Picaud, Paul N. M. Hoang

▶ To cite this version:

> Stéphanie Lucas, Daniel Ferry, Benjamin Demirdjian, Jean Suzanne, Sylvain Picaud, et al.. Dynamics of ice Ih films upon methanol adsorption : quasielastic neutron scattering experiments and molecular dynamics simulations. 11th International Conference on the Physics and Chemistry of Ice (PCI-2006), Jul 2006, Bremerhaven, Germany. hal-03691102

HAL Id: hal-03691102
https://hal.science/hal-03691102

Submitted on 19 Oct 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Distributed under a Creative Commons Attribution 4.0 International License

DYNAMICS OF ICE IH FILMS UPON METHANOL ADSORPTION: QUASIELASTIC NEUTRON SCATTERING EXPERIMENTS AND MOLECULAR DYNAMICS SIMULATIONS

S. Lucas[1], D. Ferry[1], B. Demirdjian[1], J. Suzanne[1], S. Picaud[2] and P. N. M. Hoang[2]

(1) CRMC-N, UPR CNRS 7251, Campus de Luminy, Case 913, F-13288 Marseille Cedex 09 - France.

(2) Laboratoire de Physique Moléculaire, UMR CNRS 6624, Université de Franche-Comté, F-25030 Besançon Cedex - France

Introduction

[illegible]

Experiments

Experimental set-up and sample preparation

[illegible]

[illegible]

[illegible]

[illegible]

Incoherent quasielastic neutron scattering model

[illegible]

Fitting procedure and results

[illegible]

[illegible]

[illegible]

[illegible]

Molecular dynamics simulations

Details of the simulations

- ✓ Standard NVT molecular dynamics simulations are performed between 200 and 270 K.
- ✓ The simulation box contains 768 water molecules adsorbed on a rigid MgO substrate.
- ✓ Various coverages of methanol are deposited on the ice surface.
- ✓ The timestep is 2.5 fs.
- ✓ Long runs have been performed: 1500 ps of equilibration + 200 ps of production.
- ✓ TIP5P potential for water-water interactions (3).

Structural results

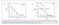
[illegible]

[illegible]

Dynamical results

[illegible]

[illegible]



[illegible]

Conclusions

We have combined quasielastic neutron scattering experiments to molecular dynamics simulations to study the dynamics of the methanol/ice/MgO system between 200 and 270 K.

[illegible]

References

[illegible]