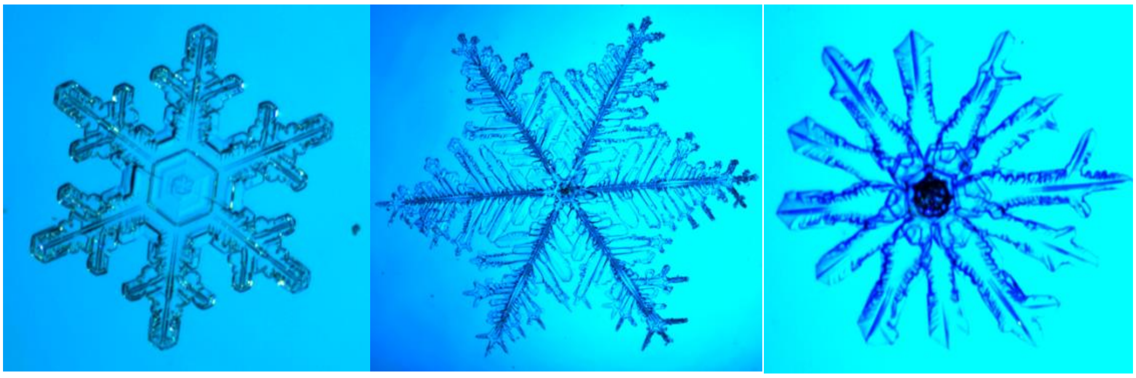
PCI-2023

The 15th International Conference
on the Physics and Chemistry of Ice

September 3-8, 2023

Conference Hall, Hokkaido University,
Sapporo, Japan

Abstracts



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Abstracts

PCI-2023

The 15th International Conference on the Physics and Chemistry of Ice (PCI-2023) is held at the Conference Hall on the campus of Hokkaido University, located in the center of Sapporo. PCI meetings were previously held in 1966, 1991, and 2010 in Sapporo. The PCI-2023 is the fourth conference held in Sapporo. We are proud of organizing the PCI-2023 conference at Hokkaido University, where Prof. Ukichiro Nakaya succeeded in growing artificial snow crystals for the first time in 1936 and since then many pioneering studies were performed on snow and ice.

Scientific Committee

Katrin Amann-Winkel (Germany / Sweden)
Ian Baker (USA)
Thorsten Bartels-Rausch (Switzerland)
Werner F. Kuhs (Germany)
Maurine Montagnat (France)
Hiroki Nada (Japan)
Jan Pettersson (Sweden)
Gen Sazaki (Japan)
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Tsutomu Uchida (Hokkaido University)
Naoki Watanabe (Hokkaido University)
Tomoya Yamazaki (Hokkaido University)
Yoshinori Furukawa (Hokkaido University), Advisor

General Information

Conference Desk

The Conference Desk is in the Foyer (1st floor) of the Conference Hall of Hokkaido University. The opening hours will be as follows:

Monday, September 4:	12:00-19:00
Tuesday, September 5:	08:30-19:00
Wednesday, September 6:	08:30-13:30
Thursday, September 7:	08:30-18:10
Friday, September 8:	08:30-12:00

Scientific Program

There will be one plenary talk, nine invited talks, and 80 contributed talks for scientific oral sessions. We will also have 39 poster presentations for two poster sessions.

Badges

Your badge serves as evidence of registration and administration. Therefore, please wear it during all scientific and social events for security and catering information as well.

Oral Presentations

Oral Presentations except for plenary and invited talks will be 20-min long including 5-min discussion times. A plenary talk will be 40-min including a 5-min discussion and invited talks will be 30-min including 5-min discussions. Please prepare your presentations accordingly.

An LCD projector and a Windows PC with Microsoft PowerPoint are available for presentations in each lecture room. The PowerPoint files for oral presentations should be installed on the PC and confirmed its operation without problems. You can also use your own PCs. In that case, you must prepare the adapter to connect with the HDMI connector and check the connection between your PC and the projector before the session starts. Note that time lost between switching PCs or due to non-functioning PCs will be deducted from the allotted presentation time. If you need any other device, please contact the organizers in advance.

Poster Presentations

Posters will be on display in the Foyer (1st floor) of the Conference Hall. The size of posters must not exceed 90 cm wide by 180 cm high. There are two poster sessions on

Tuesday afternoon (Poster Session 1 for odd-number presentations) and Thursday afternoon (Poster Session 2 for even-number presentations). Posters must be mounted before Poster Session 1 and dismounted before 9:00 on Friday. The presenting authors are expected to be in front of the posters during the poster session. The organizers are not responsible for any lost posters. Any posters left after closing will be disposed of if not claimed.

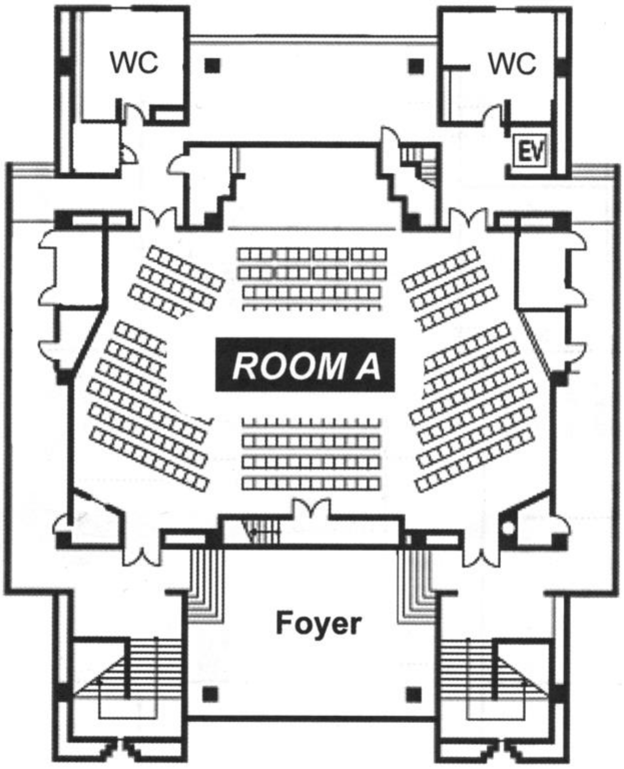
Social Events and Activities *(Not available for on-site-registration attendees)*
Sunday, September 3, 17:00-19:00: **The welcome party** at Hotel Mystays Sapporo Aspen (see the map on the back cover of this book). A fee is included in the conference registration fee. Light meals, snacks, and drinks will be provided. Accompanying guests are also welcome to attend the party.

Wednesday, September 6, 13:30-18:00: **Excursion**. Two courses are arranged for the half-day bus tours. Course A: Otaru City Tour, and Course B: Sapporo City Tour. The busses for both courses will leave in front of the Conference Hall at exactly 13:30. By 13:30 please finish your lunch or prepare your lunch to eat on the bus. After finishing the excursion, all the participants will get together at Hotel Mystays Sapporo Aspen for the banquet. A fee is included in the conference registration fee.

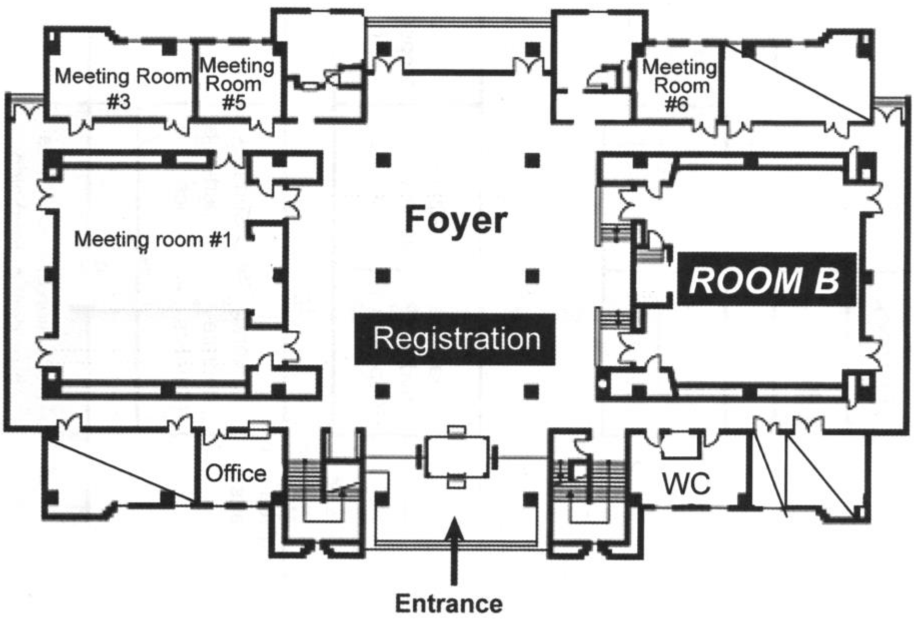
Wednesday, September 6, 18:00-20:00: **PCI-2023 Banquet** at Hotel Mystays Sapporo Aspen (see the map on the back cover of this book). A fee is included in the conference registration fee.

Access from New Chitose Airport to the Conference Hall of Hokkaido University
There are several ways of transportation from New Chitose Airport to Sapporo. The most convenient way is to take the JR (Japan Railway) trains from New Chitose Airport Station to Sapporo Station. Rapid trains (called “Rapid Airport Express”) are available approximately every 15 minutes except in the early morning and late evening. The one-way ride takes about 40 minutes and costs 1,150 JPY.
From JR Sapporo station to the Conference Hall of Hokkaido University, it takes about 10 minutes on foot. For details, see the map on the back cover of this book.

Floor Maps of the Conference Hall of Hokkaido University



2nd Floor



1st Floor

The 15th International Conference on the Physics and Chemistry of Ice (PCI-2023)

Names in red show chairpersons.

	Sept. 3 (Sun)	Sept. 4 (Mon)		Sept. 5 (Tue)		Sept. 6 (Wed)		Sept. 7 (Thu)		Sept. 8 (Fri)	
		Room A	Room B	Room A	Room B	Room A	Room B	Room A	Room B	Room A	Room B
9:00				Hiroki Nada Crystal growth of ice 1	Tsutomu Uchida Clathrate hydrates 1	Kim Kyung Hwan Ice phases, amorphous ice and glass transition 2	Xiangrui Kong Reactions on/in ice 2	Livia Bove Ice phases, amorphous ice and glass transition 4		Not available	Kenji Mochizuki Theoretical and computational works on ice 1
10:00				Luis MacDowell Crystal growth of ice 2	Hideo Tajima Clathrate hydrates 2	Osamu Yamamuro Ice phases, amorphous ice and glass transition 3	Patric Ayotte Reactions on/in ice 3	Chao Qi Mechanical, dielectric, and optical properties of ice 1	Ido Braslavsky Ice and life 1		Masakazu Matsumoto Theoretical and computational works on ice 2
11:00											Closing
12:00											
13:00		Openning Gen Sazaki Plenary		Kevin Hammonds Crystal growth of ice 3	Yongwon Seo Clathrate hydrates 3	Excursion		Ian Baker Mechanical, dielectric, and optical properties of ice 2	Tatsuya Arai Ice and life 2		
14:00		Emily Asenath-Smith Surfaces and interfaces of ice 1	Robert Style Ice and snow in the cryosphere 1					Ayobami Ogunmolasuy			
15:00				Katrin Amann-Winkel Ice phases, amorphous ice and glass transition 1	Kitae Kim Reactions on/in ice 1			Mechanical, … ice 3			
16:00		Shultz Mary Jane Surfaces and interfaces of ice 2	Frederic Flin Ice and snow in the cryosphere 2					Poster session 2 (Even numbers)			
17:00	Welcome party at Hotel Mystays Sapporo Aspen	Hiromasa Niinomi Surfaces and Interfaces of ice 3	Erik Thomson Ice and snow in the cryosphere 3	Poster session 1 (Odd numbers)							
18:00						Banquet at Hotel Mystays Sapporo Aspen					
19:00											
20:00											

September 3, Sunday

17:00-19:00 **Welcome party** **Hotel Mystays Sapporo Aspen**

September 4, Monday

12:00-13:30 **Registration** **Lobby (Foyer)**

13:30-13:40 **Opening** **Room A**

13:40-14:20 **A Plenary Lecture** **Room A**

Chairperson: Gen Sazaki

13:40-14:20 4-A1-1 **Physicochemical Processes of OH Radicals on Ice at Low Temperatures**
Naoki Watanabe[1]
[1] Institute of Low Temperature Science, Hokkaido University, N19-W8, Kita-ku, Sapporo 060-0819, Japan

14:40-15:50 **Surfaces and Interfaces of Ice 1** **Room A**

Chairperson: Emily Asenath-Smith

14:40-15:10 4-A2-1 **Ice Faces: A Molecular View of Growth and Interactions (Invited)**
Mary Jane Shultz[1], Emma Gubbins[1], Ziqing Xiong[1], Sahar Shata[1]
[1] Tufts University

15:10-15:30 4-A2-2 **In-Situ Observations of Low- and High-Density Unknown Waters at Interfaces between Water and Ices Grown/Melted by Pressure**
Hiromasa Niinomi[1], Tomoya Yamazaki[2], Hiroki Nada[3], Tetsuya Hama[4], Akira Kouchi[2], Tomoya Oshikiri[1,5], Masaru Nakagawa[1], Jun Nozawa[6], Satoshi Uda[7], Yuki Kimura[2]
[1] Institute of Multidisciplinary Research for Advanced Materials, Tohoku University,
[2] Institute of Low Temperature Science, Hokkaido University
[3] Faculty of Engineering, Tottori University
[4] Komaba Institute for Science, Tokyo University
[5] Research Institute for Electronic Science, Hokkaido University
[6] Institute for Materials Research, Tohoku University
[7] New Industry Creation Hatchery Center, Tohoku University

15:30-15:50 4-A2-3 **Measurements of Negative Surface Voltage Variation of Amorphous Solid Water with a Nanoscale Spatial Resolution by FM-AFM**
Takuto Tomaru[1], Hiroshi Hidaka[1], Naoki Watanabe[1]
[1] Institute of Low Temperature Science, Hokkaido University

16:10-17:10 **Surfaces and Interfaces of Ice 2 Room A**

Chairperson: Shultz Mary Jane

16:10-16:30 4-A3-1 **Polycrystallinity Significantly Enhances Stress Build-Up During Freezing**
Dominic Gerber[1], Lawerence A. Wilen[2], Erice R. Dufresne[1], Robert Style[1]
[1] Soft and Living Materials, Department of Materials, ETH Zürich, 8093 Zürich, Switzerland
[2] Center for Engineering Innovation and Design, School of Engineering and Applied Sciences, Yale University, New Haven, Connecticut 06520, USA

16:30-16:50 4-A3-2 **Growth and Form of Rippled Icicles**
Menno Demmenie[1,2], Lars Reus[1], Paul Kolpakov[1], Sander Woutersen[2], Daniel Bonn[1], Noushine Shahidzadeh[1]
[1] Institute of Physics, University of Amsterdam, Science Park 904, Amsterdam 1098 XH, Netherlands
[2] Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, Amsterdam 1098XH, Netherlands

16:50-17:10 4-A3-3 **Ice Removal from Surfaces by Interfacial Crack Propagation**
Emily Asenath-Smith[1], Olivier Montmayeur[1], Travis Hilton[1], Jeffrey Allen[2], Robert Haehnel[1]
[1] Cold Regions Research and Engineering Laboratory (CRREL), US Army Corps of Engineers Engineer Research & Development Center, 72 Lyme Road, Hanover NH, 03755, United States of America
[2] Information Technologies Laboratory, US Army Corps of Engineers Engineer Research & Development Center 3909 Halls Ferry Road, Vicksburg, MS 39180, United States of America

17:30-18:10 **Surfaces and Interfaces of Ice 3 Room A**

Chairperson: Hiromasa Niinomi

17:30-17:50 4-A4-1 **Hydrogen Bonding in Water Enhanced by Local Electric Field in Polyelectrolyte Brushes**
Yoshihisa Harada[1], Kosuke Yamazoe[2], Yuji Higaki[3], Jun Miyawaki[4], Atsushi Takahara[5]
[1] Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba 277-8581, Japan
[2] Japan Synchrotron Radiation Research Institute, Sayo, Hyogo 679-5198, Japan
[3] Department of Integrated Science and Technology, Faculty of Science and Technology, Oita University, Dannoharu, Oita 870-1192, Japan
[4] National Institutes for Quantum Science and Technology (QST), Aoba-ku, Sendai, Miyagi 980-8572, Japan
[5] Research Center for Negative Emission Technologies, Kyushu University, Nishi-ku, Fukuoka 819-0395, Japan

17:50-18:10 4-A4-2 **Adsorption Structures of Ammonia Molecules on Crystalline Ice**
Du Hyeong Lee[1,2], Heon Kang[2]
[1] Korea Polar Research Institute
[2] Seoul National University

14:40-15:50 Ice and Snow in the Cryosphere 1 Room B

Chairperson: Robert Style

14:40-15:10 4-B2-1 **Measuring Microscale Mechanisms of Snow Melt, Rain-on-Snow, Drainage, and Imbibition Using Rapid Magnetic Resonance Profiling (Invited)**
Quirine Krol[1,2], Sarah Codd[1], Kevin Hammonds[2], Matthew Skuntz[1], Joseph D. Seymour[1]
[1] Magnetic Resonance Laboratory, Montana State University
[2] Subzero Laboratory, Montana State University

15:10-15:30 4-B2-2 **Ice Particles in Clouds: Origins, Processing, and Cloud Lifetime**
Erik S. Thomson[1], Luisa Ickes[2], Luis F.E.d. Santos[1], Hannah C. Frostenberg[2]
[1] Department of Chemistry and Molecular Biology, University of Gothenburg, Gothenburg 41296, Sweden
[2] Department of Space, Earth and Environment, Chalmers University, Gothenburg 41296, Sweden

15:30-15:50 4-B2-3 **Direct Observation of Wet Snow Using X-Ray Tomography: First Results and Outlooks**
Frederic Flin[1], Pierre Latil[1], Iheb Haffar[1], Laurent Pezard[1], Jacques Roulle[1], Hayat Benkhelifa[2,3], Pascal Charrier[4], Nicolas Lenoir[4], Fatou-Toutie Ndoye[2], Jonathan Perrin[5], Mario Scheel[5], Timm Weitkamp[5]
[1] Univ. Grenoble Alpes, Universite de Toulouse, Meteo-France, CNRS, CNRM, Centre d'Etudes de la Neige, Grenoble, France
[2] Universite Paris-Saclay, INRAE, UR FRISE, F-92761 Antony, France
[3] Universite Paris-Saclay, INRAE, AgroParisTech, 75005 Paris, France
[4] Universite Grenoble Alpes, Grenoble INP, 3SR, CNRS, Grenoble, France
[5] Synchrotron SOLEIL, 91190 Saint-Aubin, France

16:10-17:10 Ice and Snow in the Cryosphere 2 Room B

Chairperson: Frederic Flin

16:10-16:30 4-B3-1 **Pattern Formation of Refrozen Melt Structures in Snowpack**
Nathan Jones[1], Adrian Moure[1], Xiaojing Fu[1]
[1] Department of Mechanical and Civil Engineering, California Institute of Technology, 1200 E California Blvd., Pasadena, CA 91125, USA

16:30-16:50 4-B3-2 **A Physical Model of Gas Bubble Nucleation and Transport in Sea Ice**
Joseph Fishlock[1], Andrew Wells[1], Christopher MacMinn[2]
[1] Atmospheric, Oceanic & Planetary Physics, Dept. of Physics, University of Oxford
[2] Dept. of Engineering Science, University of Oxford

16:50-17:10 4-B3-3 **Effects of Sulfuric Acid on Sintering of Laboratory Simulated Polar Firn**
Evan N. Schehrer[1], Marika Feduschak[1], Khristian Jones[1], Kevin Hammonds[1]
[1] Montana State University, Subzero Research Laboratory, Bozeman, MT, USA

17:30-18:50 **Ice and Snow in the Cryosphere 3** **Room B**

Chairperson: Erik Thomson

17:30-17:50 4-B4-1 **Investigation of Structure and Geochemical Composition of Ushkovsky Shallow Ice Core**
Mstislav Vorobyev[1], Vladimir Mikhalenko[1], Aleksandra Khairedinova[1], Julia Chizhova[1,2], Maria Vinogradova[1]
[1] Institute of Geography, Russian Academy of Sciences, Glaciology, Moscow, Russia
[2] Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry, Russian Academy of Science, Moscow, Russia

17:50-18:10 4-B4-2 **Ice-Drilling Method of Continuously Coring with Air Reverse Circulation**
Rusheng Wang[1], Xinyu Lv[1], Zhihao Cui[1]
[1] Polar Research Center, Jilin University

18:10-18:30 4-B4-3 **International Efforts and Chinese Contributions on Mapping Subglacial Topography of the Antarctica Ice Sheet**
Xiangbin Cui[1]
[1] Polar Research Institute of China

18:30-18:50 4-B4-4 **Freezing Damage in Brittle Hydrogels**
Shaohua Yang[1], Dominic Gerber[2], Nicolas Bain[2], Laura de Lorenzis[2], Eric Dufresne[2,3], Robert Style[2]
[1] Beihang University, Beijing, 100191, China
[2] ETH Zürich, Zürich, 8093, Switzerland
[3] Cornell University, Ithaca, NY 14850, USA

September 5, Tuesday

9:00-10:10 **Crystal Growth of Ice 1** **Room A**

Chairperson: Hiroki Nada

9:00-9:30 5-A1-1 **Step-Bunching Instability of Growing Interfaces between Ice and Supercooled Water (Invited)**
Ken-ichiro Murata[1], Masahide Sato[2], Makio Uwaha[3], Fumiaki Saito[1], Ken Nagashima[1], Gen Sazaki[1]
[1] Institute of Low Temperature Science, Hokkaido University, N19-W8, Kita-ku, Sapporo 060-0819, Japan
[2] Emerging Media Initiative, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan
[3] Center for General Education, Aichi Institute of Technology, Yakusa-cho, Toyota 470-0392, Japan

9:30-9:50 5-A1-2 **Liquid-Cell Transmission Electron Microscopy of Ice Crystals and Bubble Behaviors in the Ice**
Tomoya Yamazaki[1], Yuga Yashima[1], Hiroyasu Katsuno[1], Hiroya Miyazaki[2], Takashi Gondo[2], Yuki Kimura[1]
[1] Institute of Low Temperature Science, Hokkaido University
[2] Mel-Build Corporation

9:50-10:10 5-A1-3 **Characterizing Faceted Snow Crystals with Electron Backscatter Diffraction**
Evan N. Schehrer[1], Kevin Hammonds[1]
[1] Montana State University, Subzero Research Laboratory, Bozeman, MT, USA

10:30-11:50 Crystal Growth of Ice 2 Room A

Chairperson: Luis MacDowell

10:30-10:50 5-A2-1 **Microscopic Ordering of Supercooled Water on the Ice Basal Face**
Kenji Mochizuki[1], Ken-ichiro Murata[2], Xuan Zhang[1]
[1] Department of Chemistry, Zhejiang University, Hangzhou, 310028, P. R. China
[2] Institute of Low Temperature Science, Hokkaido University, N19-W8, Kita-ku, Sapporo 060-0819, Japan

10:50-11:10 5-A2-2 **Effect of Air Molecules on the Growth Kinetics of Ice from Water Studied by Molecular Dynamics Simulation**
Hiroki Nada[1]
[1] Tottori University

11:10-11:30 5-A2-3 **Toward the Rational Design of Novel Cryoprotectants**
Gabriele C. Sosso[1], Fabienne Bachtiger[1], Matthew T. Warren[1], Matthew I. Gibson[1]
[1] Department of Chemistry, University of Warwick, CV4 7AL, Coventry, United Kingdom

11:30-11:50 5-A2-4 **A Self-Oscillatory Growth Model of an Ice Crystal in Antifreeze Glycoprotein Solution**
Etsuro Yokoyama[1]
[1] Gakushuin University

13:30-15:10 Crystal Growth of Ice 3 Room A

Chairperson: Kevin Hammonds

13:30-13:50 5-A3-1 **Surface Phase Transitions, Anomalous Step Free Energies and Crystal Growth Rates of Ice in the Atmosphere**
Pablo Llombart[1,2], Eva G. Noya[3], Luis G. MacDowell[1]
[1] Universidad Complutense de Madrid, Spain.
[2] Instituto de Física Nicolás Cabrera, Madrid, Spain.
[3] Instituto de Química Física Rocasolano, Madrid, Spain.

13:50-14:10 5-A3-2 **Temperature Dependence of the Growth Kinetics of Elementary Spiral Steps on Ice Prism Faces Grown in Vapor**
Genki Miyamoto[1], Akira Kouchi[1], Ken-ichiro Murata[1], Ken Nagashima[1], Gen Sazaki[1]
[1] Institute of Low Temperature Science, Hokkaido University

14:10-14:30 5-A3-3 **Uptake Mechanism of Atmospheric-Concentration HCl Gas in Ice Crystals via Hydrochloric Acid Droplets**
Ken Nagashima[1], Ken-ichiro Murata[1], Gen Sazaki[1]
[1] Institute of Low Temperature Science, Hokkaido University, Japan

14:30-14:50 5-A3-4 **Quantification of Anion and Cation Uptake in Ice Ih Crystals**

Jenee D. Cyran[1,2], Tiara Sivellls[2], Pranav Viswanathan[2]

[1] Boise State University

[2] Baylor Univeristy

14:50-15:10 5-A3-5 **Solute Interactions in Ice: Color Quenching and Crystallization Effects**

Daniel W. Tague[1], Timothy Schutt[2], Manoj Shukla[2], Gilbert Kosgei[2], Emily Asenath-Smith[1]

[1] Cold Regions Research and Engineering Laboratory, US Army Corps of Engineers Engineer Research & Development Center, 72 Lyme Road, Hanover NH, 03755, United States of America

[2] Environmental Laboratory, US Army Corps of Engineers Engineer Research & Development Center 3909 Halls Ferry Road, Vicksburg, MS 39180, United States of America

15:30-16:40 Ice Phases, Amorphous Ice, and Glass Transition 1 Room A

Chairperson: Katrin Amann-Winkel

15:30-16:00 5-A4-1 **Ultrafst Melting and Recrystallization Dynamics of Ice Revealed by Time-Resolved X-Ray Scattering at FELs (Invited)**

Kyung Hwan Kim[1]

[1] Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, Gyeongbuk 37673, Republic of Korea.

16:00-16:20 5-A4-2 **Cooperative Molecular Dynamics of High-Density Water; Dielectric Study on Glycerol Water Mixtures Under High Pressure**

Kaito Sasaki[1,2,3], Yoshiharu Suzuki[3]

[1] Department of Physics, Tokai University, Kitakaname 4-1-1, Hiratsuka, Kanagawa 259-1292, Japan.

[2] Micro/Nano Technology Center, Tokai University, Kitakaname 4-1-1, Hiratsuka, Kanagawa 259-1292, Japan.

[3] Research Center for Advanced Measurement and Characterization, National Institute for Materials Science (NIMS), Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan

16:20-16:40 5-A4-3 **Neutron Diffraction Study of the Hydrogen-Bond Symmetrization in Ice**

Kazuki Komatsu[1], Stefan Klotz[2], Shinichi Machida[3], Takanori Hattori[4], Asami Sano-Furukawa[4], Keishiro Yamashita[1,5], Hiroki Kobayashi[1], Hayate Ito[1], Hiroyuki Kagi[1]

[1] Geochemical Research Center, Graduate School of Science, The University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-0033, Japan

[2] IMPMC, CNRS UMR 7590, Sorbonne Université, 4 Place Jussieu, F-75252 Paris, France

[3] Neutron Science and Technology Center, CROSS, 162-1 Shirakata, Tokai, Ibaraki 319-1106, Japan

[4] J-PARC Center, Japan Atomic Energy Agency, 2-4 Shirakata, Tokai, Ibaraki 319-1195, Japan

[5] Institute of Physical Chemistry, University of Innsbruck, A-6020 Innsbruck, Austria

9:00-10:10 Clathrate Hydrates 1 Room B

Chairperson: Tsutomu Uchida

9:00-9:30 5-B1-1 **Exploring the Stability and New Structures of Gas Filled Ices Up to Mbar Pressures (Invited)**
Umbertoluca Ranieri[1], Simone Di Cataldo[1], Lorenzo Monicelli[2], Maria Rescigno[1,2], Richard Gaal[2], Livia E. Bove[1,2,3]
[1] Università di Roma La Sapienza, Roma, Italy
[2] LQM, EPFL, Lausanne Switzerland
[3] CNRS UMR7590, Paris, France

9:30-9:50 5-B1-2 **Ammonia and Clathrate Hydrates: Phase Behavior and Structural Implications, Including Incorporation**
Mathieu Choukroun[1], Elodie Gloesener[1], Tuan H. Vu[1], Helen E. Maynard-Casely[2], Ashley G. Davies[1], Arnaud Desmedt[3], Christophe Sotin[4]
[1] Jet Propulsion Laboratory, California Institute of Technology
[2] Australia's Nuclear Science and Technology Organization
[3] Institut des Sciences Moléculaires, CNRS UMR 5255, Talence, France
[4] Laboratoire de Planétologie et Géosciences, CNRS UMR 6112, Nantes, France

9:50-10:10 5-B1-3 **Methane – Ethane Substitution in Clathrate Hydrates Studied by Raman Spectroscopy: Implications for the Carbon Cycle on Titan**
Elodie Gloesener[1], Tuan H. Vu[1], Mathieu Choukroun[1], Ashley G. Davies[1], Arnaud Desmedt[2], Christophe Sotin[3]
[1] Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, United States
[2] Institut des Sciences Moléculaires, CNRS UMR 5255, Talence, France
[3] Nantes Université, Laboratoire de Planétologie et Géosciences, CNRS UMR 6112, Nantes, France

10:30-11:50 Clathrate Hydrates 2 Room B

Chairperson: Hideo Tajima

10:30-10:50 5-B2-1 **Complete Low Pressure (80 bar) Cycling of Hydrogen in Pure Hydrogen Hydrate: Toward Gas Storage**
Chris A. Tulk[1], Jamie Molaison[1], Dennis Klug[2]
[1] Oak Ridge National Laboratory
[2] National Research Council of Canada

10:50-11:10 5-B2-2 **Formation of Mixed Hydrate to Separate CO_2 from R134a + CO_2 Gas Mixture for LNG Gasification Unit**
Yutaek Seo[1]
[1] Seoul National University

11:10-11:30 5-B2-3 **Effect of Injecting Pressure on CO_2 Exchange Behaviors into C_3H_8 Hydrate**
Jonghyuk Lee[1], Junghoon Mok[1,2], Wonjung Choi[3], Seongju Mun[4], Yongwon Seo[1,4,5]
[1] Department of Urban and Environmental Engineering, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea
[2] Department of Chemical and Biological Engineering, Colorado School of Mines, CO 80401, USA
[3] Department of Chemical Engineering, Changwon National University, Gyeongnam 51140, Republic of Korea

[4] Graduate School of Carbon Neutrality, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea
[5] Corresponding Author

11:30-11:50 5-B2-4 **Crustal Fingering Facilitates Free-Gas Methane Migration Through the Hydrate Stability Zone**
Xiaojing Fu[1]
[1] California Institutte of Technology

13:30-15:10 **Clathrate Hydrates 3** **Room B**

Chairperson: Yongwon Seo

13:30-13:50 5-B3-1 **On the Thermodynamic Stability of CH_4-CO_2 Binary Hydrates Under Multiple Coexistence of Water, Hydrate, and Guest Fluids.**
Hideki Tanaka[1]
[1] Toyota Physical and Chemical Research Institute

13:50-14:10 5-B3-2 **Metastability of Carbon Monoxide and Nitrogen Gas Hydrates from First-Principles Calculations**
Ludovic Martin-Gondre[1], Claire Pétuya[2], Cyrielle Métais[1,2,3], Jacques Ollivier[3], Arnaud Desmedt[2]
[1] UTINAM Institute, UMR6213 CNRS – Univ. Franche-Comté, Besançon, France
[2] ISM, UMR5255 CNRS – Univ. Bordeaux, Fran
[3] Institut Laue Langevin, Grenoble, France

14:10-14:30 5-B3-3 **Rotations of Methane Molecules in Amorphous and Crystalline Hydrates**
Menghan Zhang[1], Hiroshi Akiba[1], Osamu Yamamuro[1]
[1] Institute for Solid State Physics, University of Tokyo

14:30-14:50 5-B3-4 **Proton Conduction Mechanism in TBAB Semiclathrate Hydrate Obtained by NMR and QENS Measurements**
Jin Shimada[1], Takeshi Sugahara[1], Atsushi Tani[2], Takahiro Ueda[3], Takeshi Yamada[4], Takuo Okuchi[5], Katsuhiko Tsunashima[6], Takayuki Hirai[1]
[1] Graduate School of Engineering Science, Osaka University
[2] Graduate School of Human Development and Environment, Kobe University
[3] Graduate School of Science, Osaka University
[4] Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society
[5] Institute for Integrated Radiation and Nuclear Science, Kyoto University
[6] National Institute of Technology, Wakayama College

14:50-15:10 5-B3-5 **Homogeneous and Heterogeneous Nucleation of Clathrate Hydrates Under Non-Equilibrium Conditions with Time and Temperature Resolved Synchrotron X-Ray Diffraction**
John S. Tse[1], Robert Bauer[1]
[1] Department of Physics and Engineering Physics
[2] University of

15:30-16:40 **Reactions on/in Ice 1** **Room B**

Chairperson: Kitae Kim

15:30-16:00 5-B4-1 **Insights from Structure and Chemical Reactivity of Water Adsorbed on Particle Surfaces (Invited)**

Xiangrui Kong[1], Ivan Gladich[2,3], Nicolas Fauré[1], Erik S. Thomson[1], Luca Artiglia[4], Markus Ammann[4], Thorsten Bartels-Rausch[4], Jan Pettersson[1]

[1] Department of Chemistry and Molecular Biology, Atmospheric Science, University of Gothenburg, SE-41296 Gothenburg, Sweden

[2] European Centre for Living Technology (ECLT), Dorsoduro, Calle Crosera, 30124 Venice, Italy

[3] Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. Box 31110, Doha, Qatar

[4] Laboratory of Environmental Chemistry, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

16:00-16:20 5-B4-2 **Experimental Characterization of the NO_2/N_2O_4 Hydrolysis Reaction Intermediates on Ice**

Josée Maurais[1], Clément Wespiser[1], Patrick Ayotte[1]

[1] Université de Sherbrooke, Département de chimie, 2500 Boul. de l'université, Sherbrooke (Qc)

16:20-16:40 5-B4-3 **Isotopic Constraints on Snow Nitrate Photolysis in Inland East Antarctica: Knowns and Unknowns**

Guitao Shi[1], Aron M. Buffen[2], Ye Hu[1], Meredith G. Hastings[2]

[1] East China Normal University

[2] Brown University

17:00-19:00 **Poster Session 1 (Odd Numbers)** **Lobby (Foyer)**

Posters with odd numbers are presented.

September 6, Wednesday

9:00-10:20 **Ice Phases, Amorphous Ice, and Glass Transition 2** **Room A**

Chairperson: Kim Kyung Hwan

9:00-9:20 6-A1-1 **Polyamorphism in Vitrified Water Droplets: Nucleation of a Liquid in a Liquid**

Johannes Bachler[1], Johannes Giebelmann[1], Thomas Loerting[1]

[1] Institute of Physical Chemistry, University of Innsbruck, Innrain 52c, 6020 Innsbruck, Austria

9:20-9:40 6-A1-2 **Revealing the Dynamics of High-Density Amorphous Ice Using X-Ray Photon Correlation Spectroscopy**

Hailong Li[1,4], Marjorie Ladd-Parada[2], Aigerim Karina[2], Katrin Amann-Winkel[1,2,3]

[1] Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

[2] Department of Physics, Stockholm University, Roslagstullsbacken 21, 10691 Stockholm, Sweden

[3] Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

[4] Department of Polymer Science & Materials, Dalian University of Technology, Dalian 116024, PR China

9:40-10:00 6-A1-3 **Topological Analysis on Amorphous Ices Using Persistent Homology**
Hayate Ito[1], Kazuki Komatsu[1]
[1] Geochemical Research Center, Graduate School of Science, The University of Tokyo,

10:00-10:20 6-A1-4 **Structure and Phonon Excitations of Vapor-Deposited Amorphous Ice and Their Annealing Effects Studied by X-Ray/Neutron Scattering Techniques**
Osamu Yamamuro[1], Masashi Kunizawa[1], Xuejun Wu[1], Hiroshi Akiba[1], Kazutaka Ikeda[2], Maiko Kofu[3]
[1] Institute for Solid State Physics, University of Tokyo
[2] Institute of Materials Structure Science, High Energy Accelerator Research Organization
[3] J-PARC Center, Japan Atomic Energy Agency

10:40-11:40 Ice Phases, Amorphous Ice, and Glass Transition 3 Room A

Chairperson: Osamu Yamamuro

10:40-11:00 6-A2-1 **In-Situ Observation of Pressure-Induced Amorphization of Methane/Ethane Hydrates by Vibrational Spectroscopy**
Naoki Noguchi[1], Yui Shiraishi[1], Maho Kageyama[1], Yuu Yokoi[1], Saki Kurohama[1], Natsuki Okada[1], Hidekazu Okamura[1]
[1] Graduate School of Technology, Industrial and Social Sciences, Tokushima University

11:00-11:20 6-A2-2 **A Systematic Study of the Influence of the Ice Formation Temperature on Spectroscopic Properties of Methanol Interstellar Ice Analogues**
Marta E. Podgórny[1], Anita Dawes[1]
[1] School of Physical Sciences, The Open University, Walton Hall, Milton Keynes, MK7 6AA, United Kingdom

11:20-11:40 6-A2-3 **Accurate Crystal Structures of Ices from X-Ray and Electron Diffraction with Hirshfeld Atom Refinement**
Krzysztof Wozniak[1], Michal Chodkiewicz[1], Roman Gajda[1], Vitali Prakapenka[2], Przemyslaw Dera[3]
[1] University of Warsaw, Chemistry Department, Pasteura 1, 02093 Warszawa, Poland
[2] APS, Argonne National Laboratory, 9700 South Cass Avenue, Lemont, IL 60439, USA
[3] Hawai'i Institute of Geophysics and Planetology, Université d'hawaï à mānoa, 1680 East-West Road, Honolulu, HI 96822, USA

9:00-10:20 Reactions on/in Ice 2 Room B

Chairperson: Xiangrui Kong

9:00-9:20 6-B1-1 **The Inherent Chemical Reactions Occurring Within Ice and Their Consequential Implications and Potential Applications**
Kitae Kim[1,2]
[1] Korea Polar Research Institute
[2] Department of Polar Science, University of Science and Technology

9:20-9:40 6-B1-2 **Quantitative Study of Freezing Concentration in Polycrystalline Ice Crystals upon Ice Recrystallization**
Bomi Kim[1], Kitae Kim[1,2]
[1] Korea Polar Research Institute (KOPRI), Incheon 21990, Republic of Korea
[2] Department of Polar Sciences, University of Science and Technology (UST), Incheon /21990, Republic of Korea

9:40-10:00 6-B1-3 **TEM Study on the Evolution of Micro-Cavities in Ice by Electron Radiolysis**
Yuki Nakano[1], Yuki Kimura[1], Tomoya Yamazaki[1], Yuta Sasaki[2]
[1] Institute of Low Temperature Science, Hokkaido University
[2] SCREEN Holdings Co., Ltd

10:00-10:20 6-B1-4 **Identification of a Permanent Reservoir of Bromine in Arctic Snow in the Form of Bromate (BrO_3^-)**
Stefano Frassati[1,2], Elena Barbaro[1,2], Giulio Cozzi[1,2], Clara Turetta[1,2], Federico Scoto[3], Alfonso Saiz-Lopez[4], Kitae Kim[5], Ward van Pelt[6], Carlo Barbante[1,2], Andrea Spolaor[1,2]
[1] Ca' Foscari University of Venice, Department of Environmental Sciences, Informatics and Statistics, Venice Mestre, Italy
[2] Institute of Polar Sciences – National Research Council (CNR-ISP), Venice Mestre, Italy
[3] Institute of Atmospheric Sciences and Climate CNR-ISAC, Italy
[4] Department of Atmospheric Chemistry and Climate, Institute of Physical Chemistry Rocasolano, CSIC, Madrid, Spain
[5] d Korea Polar Research Institute (KOPRI), Incheon 21990, Republic of Korea
[6] Department of Earth Sciences, Uppsala University, Uppsala, Sweden

10:40-12:00 Reactions on/in Ice 3 Room B

Chairperson: Patric Ayotte

10:40-11:00 6-B2-1 **Methanol Production Through the Impingement of Low-Energy CH_3^+ Ions onto an Ice Surface at Low Temperature**
Yoichi Nakai[1], W.M.C. Sameera[2,3], Kenji Furuya[4], Hiroshi Hidaka[2], Atsuki Ishibashi[2], Naoki Watanabe[2]
[1] RIKEN Nishina Center for Accelerator-based Science
[2] Institute of Low Temperature Science, Hokkaido University
[3] Department of Chemistry, University of Colombo
[4] National Astronomical Observatory of Japan

11:00-11:20 6-B2-2 **Visible Light Induced Photodesorption of Hydroxyl Radicals from Amorphous Solid Water**
Masashi Tsuge[1], Ayane Miyazaki[1], Ni-En Sie[1], W.M.C. Sameera[1], Yoichi Nakai[2], Tetsuya Hama[3], Hiroshi Hidaka[1], Akira Kouchi[1], Naoki Watanabe[1]
[1] Institute of Low Temperature Science, Hokkaido University
[2] Radioactive Isotope Physics Laboratory, RIKEN Nishina Center
[3] Komaba Institute for Science, The University of Tokyo

11:20-11:40 6-B2-3 **Gas-Ice Partitioning Coefficients of Carbonyl SOA Precursors During Diffusional Ice Crystal Growth**
Jackson C. Seymore[1,2], Miklós Szakáll[2], Alexander Theis[3], Subir Mitra[3]
[1] Max Planck Graduate Center, Institute for Chemistry, Mainz, Germany
[2] Johannes Gutenberg University, Institute for Atmospheric Physics, Mainz, Germany

[3] Max Planck Institute for Chemistry, Particle Chemistry Department, Mainz, Germany

11:40-12:00 6-B2-4 **Revealing the Interfacial Dynamics Between Antifreeze Proteins and the Ice-Water Interface at Single-Molecule Level Through Subzero Nanoscopy**
Sanne Giezen[1], Ilja Voets[1,2], Roderick Tas[1,2]
[1] Technical University Eindhoven
[2] Institute for Complex Molecular Systems

13:30-18:00 **Excursion**

18:00-20:00 **Banquet** **Hotel Mystays Sapporo Aspen**

September 7, Thursday

9:00-10:20 **Ice Phases, Amorphous Ice, and Glass Transition 4** **Room A**

Chairperson: Livia Bove

9:00-9:20 7-A1-1 **Hydrogen-Ordered States of Ice V-XIII Revisited: β-State Between the Two**
Keishiro Yamashita[1], Thomas Loerting[1]
[1] Institute of Physical Chemistry, University of Innsbruck

9:20-9:40 7-A1-2 **Is a Hydrogen-Ordered Phase Corresponding to Ice IV Experimentally Accessible?**
Hiroki Kobayashi[1], Kazuki Komatsu[1], Hiroyuki Kagi[1]
[1] Geochemical Research Center, Graduate School of Science, the University of Tokyo

9:40-10:00 7-A1-3 **Ice XIX: The Second Hydrogen-Ordered Daughter Phase of Ice VI**
Tobias M. Gasser[1], Alexander Thoeny[1], Thomas Loerting[1]
[1] University of Innsbruck

10:00-10:20 7-A1-4 **Kinetics of the Hydrogen Order-to-Order Transition in Ice XV/XIX**
Alexander Thoeny[1], Tobias Gasser[1], Thomas Loerting[1]
[1] University of Innsbruck

10:40-11:50 **Mechanical, Dielectric, and Optical Properties of Ice 1** **Room A**

Chairperson: Chao Qi

10:40-11:10 7-A2-1 **The Mechanical Properties of Freshwater Ice (Invited)**
Ian Baker[1]
[1] Thayer School of Engineering, Dartmouth College

11:10-11:30 7-A2-2 **Ice Creep and Behavior of Ice Borehole**
Pavel Talalay[1,2], Jialin Hong[1]
[1] Jilin University
[2] China University of Geosciences, Beijing

11:30-11:50 7-A2-3 **Ice of H_2O with Some Additives: Experimental Observations on Mechanical Properties**
Frederik Guyon[1]
[1] Center for Scientific and Technological Studies of Aquitaine - French Atomic Energy Commission

13:30-14:50 Mechanical, Dielectric, and Optical Properties of Ice 2 Room A

Chairperson: Ian Baker

13:30-13:50 7-A3-1 **What Controls Crystallographic Preferred Orientations (Fabrics) of Deformed Ice: Constraints from Laboratory Experiments**
David J. Prior[1], Chao Qi[2], Lisa Craw[3], Andrew Cross[4], Sheng Fan[1], David Goldsby[5], Travis Hager[5], Qinyu Wang[2]
[1] University of Otago
[2] Chinese Academy of Sciences
[3] University of Tasmania
[4] Woods Hole Oceanographic Institute
[5] University of Pennsylvania

13:50-14:10 7-A3-2 **The Impacts of Impurities and Stress State on Polycrystalline Ice Deformation and Fabric Evolution**
Ayobami Ogunmolasuyi[1], Ian Baker[1]
[1] Dartmouth College

14:10-14:30 7-A3-3 **Effect of High-Pressure Sintering on Snow Density Evolution: Experiments and Results**
Jialin Hong[1], Pavel Talalay[1], Teng Man[2]
[1] Polar Research Center, College of Construction Engineering, Jilin University, Changchun 130026, China
[2] School of Engineering, Westlake University, Hangzhou, Zhejiang 310024, China

14:30-14:50 7-A3-4 **Effects of Impact Heating on Porous Icy Bodies Like Comets**
Haruka Sasai[1], Masahiko Arakawa[1], Minami Yasui[1], Kei Shirai[1]
[1] Graduate School of Science, Kobe University

15:10-15:50 Mechanical, Dielectric, and Optical Properties of Ice 3 Room A

Chairperson: Ayobami Ogunmolasuyi

15:10-15:30 7-A4-1 **Ice Multiplication Associated with Freezing of Supercooled Water Droplets**
Alexey A. Kiselev[1], Amelie Assenbaum[2], Alice Keinert[1], Thomas Leisner[1]
[1] Karlsruhe Institute of Technology, Institute of Meteorology and Climate Research, Karlsruhe, Germany
[2] Leibniz-Institute for Tropospheric Research, Leipzig, Germany

15:30-15:50 7-A4-2 **Dielectric-Infrared Spectrum of Ice and Atomic Dynamics Behind It**
Vasily Artemov[1]
[1] École Polytechnique Fédérale de Lausanne

10:40-11:50 **Ice and Life 1** **Room B**

Chairperson: Ido Braslavsky

10:40-11:10 7-B2-1 **Analysis of Antifreeze Proteins from Japanese Organisms (Invited)**
Sakae Tsuda[1]
[1] Graduate School of Frontier Sciences, The University of Tokyo

11:10-11:30 7-B2-2 **Ice-Cold and Crystal-Clear: Pinning and Surfing of Ice-Bound Antifreeze Proteins Imaged One by One with Subzero Nanoscopy**
Roderick Tas[1], Tim Hogervorst[1], Sanne Giezen[1], Daniëlle van den Broek[1], Romá Suris Valls[1], Ilja Voets[1]
[1] Eindhoven University of Technology

11:30-11:50 7-B2-3 **Observation of Dynamics of Ice-Crystals on the Surface of Antifreeze Proteins by Using Time-Resolved X-Ray Diffraction Analysis**
Tatsuya Arai[1,2], Yang Yue[1], Kazuhiro Mio[2], Sakae Tsuda[1,2], Yuji Sasaki[1,2]
[1] Graduate School of Frontier Sciences, The University of Tokyo
[2] AIST-UTokyo Advanced Operando Measurement Technology Open Innovation Laboratory (OPERANDO OIL)

13:30-14:50 **Ice and Life 2** **Room B**

Chairperson: Tatsuya Arai

13:30-13:50 7-B3-1 **Monitoring Ice Growth in Aqueous Solutions with Atomic Force Microscopy in the Presence of Ice-Binding Proteins**
Ido Braslavsky[1], Michael Chasnitsky[1], Daniel Waiger[1], Ron Tzur[1], Naomi Gillis[1], Yinon Rudich[2], Sidney R. Cohen[3]
[1] The institute of Biochemistry, Food Science, and Nutrition, The Robet H. Smith Faculty of Agricalture, Food, and Enviroment, The Hebrew University of Jerusalem, Rehovot 7610001, Israel
[2] Department of Earth and Planetary Sciences, Weizmann Institute of Science, Rehovot 7610001, Israel
[3] Department of Chemical Research Support, Weizmann Institute of Science, Rehovot 7610001, Israel.

13:50-14:10 7-B3-2 **Ice-Binding Proteins for Cryopreservation**
Daniëlle van den Broek[1,2], Tim Hogervorst[1,2], Ilja Voets[1,2]
[1] Department of Chemical Engineering and Chemistry, Laboratory of Self-Organizing Soft Matter, Eindhoven University of Technology
[2] Institute for Complex Molecular Systems, Eindhoven University of Technology

14:10-14:30 7-B3-3 **Effect of Dehydration on Cryopreservation Process using Aquaporin4-Overexpressing Cells**
Sumire Mastuo[1], Kenji Yamazaki[2], Masato Yasui[3], Youichiro Abe[3], Tsutomu Uchida[2]
[1] Graduate school of engineering, Hokkaido University, N13-W8, Kita-ku, Sapporo 060-0628, Japan
[2] Faculty of Engineering, Hokkaido University, N13-W8, Kita-ku, Sapporo 060-0628, Japan
[3] School of Medicine, Keio University, 35, Shinanomachi, Shinjuku-ku, Tokyo 160-8582, Japan

14:30-14:50 7-B3-4 **Cryopreservation of Trehalose-Transporter Expressing Cells Adhered on Glass**
Koki Watanabe[1], Takahiro Kikawada[2,3], Kenji Yamazaki[4], Tsutomu Uchida[4]
[1] Graduate School of Engineering, Hokkaido University
[2] National Agriculture and Food Research Organization (NARO)
[3] Graduate School of Frontier Sciences, The University or Tokyo
[4] Faculty of Engineering, Hokkaido University

16:10-18:10 **Poster Session 2 (Even Numbers)** **Lobby (Foyer)**

Posters with even numbers are presented.

September 8, Friday

9:00-10:10 **Theoretical and Computational Works on Ice 1** **Room B**

Chairperson: Kenji Mochizuki

9:00-9:30 8-B1-1 **The Most Potent Snow Makers (Invited)**
Valeria Molinero[1], Yuqing Qiu[1,2], Ingrid de Almeida Ribeiro[1], Konrad Meister[3,4]
[1] Department of Chemistry, The University of Utah, Salt Lake City, UT 84112, United States
[2] Department of Chemistry, University of Chicago, Chicago, Illinois 60637, United States
[3] Max Planck Institute for Polymer Research, 55128 Mainz, Germany
[4] Department of Chemistry and Biochemistry, Boise State University, Boise, Idaho 83725, United States

9:30-9:50 8-B1-2 **The Balance Principle on the Hydrogen Bond Network of Ice**
Masakazu Matsumoto[1], Takuma Yagasaki[2], Hideki Tanaka[3]
[1] Research Institute for Interdisciplinary Science, Okayama University

9:50-10:10 8-B1-3 **Confinement Effects on the o-H_2O <-> p-H_2O Nuclear Spin Isomers Interconversion Mechanism and Rates**
Patrick Ayotte[1], Thomas Putaud[1,2], Pierre-Alexandre Turgeon[1], Clément Wespiser[1], Jean-Claude Chartrand[1], Jonathan Vermette[1], Yulia Kalugina[1,3], Pierre-Nicholas Roy[3], Xavier Michaut[2]
[1] Université de Sherbrooke
[2] Sorbonne Université
[3] University of Waterloo

10:30-11:30 **Theoretical and Computational Works on Ice 2** **Room B**

Chairperson: Masakazu Matsumoto

10:30-10:50 8-B2-1 **Fast Crystal Growth of Ice VII Owing to the Decoupling of Translational and Rotational Ordering**
Xuan Zhang[1], Yifeng Yao[1], HongYi Li[2], Andre Python[2], Kenji Mochizuki[1]
[1] Department of Chemistry, Zhejiang University, Hangzhou, 310012, P. R. China
[2] School of Mathematical Sciences, Zhejiang University, Hangzhou, 310012, P. R. China

10:50-11:10 8-B2-2 **Surface Premelting of Ice Ic using Molecular Dynamics Simulation**
Ikki Yasuda[1], Noriyoshi Arai[1], Kenji Yasuoka[1]
[1] Keio University

11:10-11:30 8-B2-3 **Pore-Scale Modeling of Wet Snow Metamorphism**
Adrian Moure[1], Xiaojing Fu[1]
[1] California Institute of Technology

11:30 **Closing** **Room B**

September 5, Tuesday

17:00-19:00 **Poster session 1 (odd numbers)** **Lobby (Foyer)**

Posters with odd numbers are presented.

September 7, Thursday

16:10-18:10 **Poster session 2 (even numbers)** **Lobby (Foyer)**

Posters with even numbers are presented.

P-01 **Temperature-Dependent Dissociation Degree of Nitric Acid at the Air-Ice Interface Linked to the Hydrogen-Bonding Structure of the Ice**
Yanisha Manoharan[1], Luca Longetti[1], Luca Artiglia[1], Markus Ammann[1], Thorsten Bartels-Rausch[1]
[1] Paul Scherrer Institute

P-02 **Interactions of Small Molecules with the Growth Fronts of Ice Crystal Faces**
Emma F. Gubbins[1], Ziqing Xiong[1], Sahar Shata[1], Mary Jane Shultz[1]
[1] Labratory for Water and Surface Studies, Pearson Chemistry Laboratory, Tufts University, 62 Talbot Ave., Medford, MA 02155

P-03 **Non-Energetic Chemical Pathways of Sulfur Bearing Species with Hydrogen Atoms on Interstellar Ice**
Thanh Nguyen[1], Yasuhiro Oba[1], W.M.C. Sameera[1,2], Akira Kouchi[1], Naoki Watanabe[1]
[1] Institute of Low Temperature Science, Hokkaido University
[2] Department of Chemistry, University of Colombo

P-04 **Evolution of Crystalline Misorientations in Polycrystalline Samples of Pure Ice**
Carlos Leonardo Di Prinzio[1,2], Pastor Ignacio Achaval[1], Guillermo Andres Aguirre Varela[1,2]
[1] Facultad de Matemática Astronomía Física y Computación (FaMAF) Universidad Nacional de Córdoba, Argentina
[2] Instituto de Física "Enrique Gaviola" (IFEG) Córdoba , Argentina

P-05 **In-Situ Observation of Pit on Ice Crystal Surfaces by Confocal Optical Microscopy**
Carlos Leonardo Di Prinzio[1,2], Pastor Ignacio Achaval[1], Guillermo Andres Aguirre Varela[1,2]
[1] Facultad de Matemática Astronomía Física y Computación (FaMAF) Universidad Nacional de Córdoba (UNC), Córdoba (5000) Argentina
[2] Instituto de Física "Enrique Gaviola" (IFEG) Córdoba (5000), Argentina

P-06 **Graph Neural Networks Classify Molecular Geometry and Deign Novel Order Parameters of Ice and Water**
Satoki Ishiai[1], Katsuhiro Endo[1], Kenji Yasuoka[1]
[1] Keio university

P-07 **A Molecular Dynamics Study of Low-Angle Tilt Grain Boundary Energies in Ice Bicrystals**
Carlos Leonardo Di Prinzio[1,2], Esteban Druetta[1], Julián Roberto Fernández[3]
[1] Facultad de Matemática Astronomía Física y Computación (FaMAF) Universidad Nacional de Córdoba (UNC), Córdoba (5000) Argentina
[2] Instituto de Física "Enrique Gaviola" (IFEG) Córdoba (5000), Argentina
[3] Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), (C1425FQB) CABA, Argentina

P-08 **Side-Branch Formation and its Direction During Growth of Snow Crystals**
Wataru Shimada[1], Touma Yoshii[1], Kazuki Ohtake[1]
[1] University of Toyama

P-09 **Grain Growth with Mobile Bubbles in Ice: Experiments and Numerical Simulation**
Carlos Leonardo Di Prinzio[1,2], Pastor Ignacio Achaval[1], Guillermo Andres Aguirre Varela[1,2]
[1] Facultad de Matemática Astronomía Física y Computación (FaMAF) Universidad Nacional de Córdoba (UNC), Córdoba (5000), Argentina
[2] Instituto de Física "Enrique Gaviola" (IFEG) Córdoba (5000), Argentina

P-10 **Impact Strength of Porous Icy Bodies in High-Velocity Oblique Collision: Implication for Catastrophic Disruption of Kuiper Belt Objects in Outer Solar System**
Minami Yasui[1], Masato Nakamura[1], Masahiko Arakawa[1]
[1] Graduate School of Science, Kobe University

P-11 **Experimental Study on Collisional Disruption of Differentiated Icy Planetesimals**
Shunki Ishii[1], Yuki Eguchi[1], Minami Yasui[1], Masahiko Arakawa[1], Yukari Toyoda[1]
[1] Graduate School of Science, Kobe University

P-12 **Preliminary Results of Dielectric Profile Measurements of Ice Cores from the Flank of the Dalk Glacier, Antarctica**
Nan Zhang[1,2], Si yu Lu[1,2,3], Pavel Talalay[1,2], Yun Chen Liu[1,2], Bo Han[1,2]
[1] Construction Engineering College, Jilin University
[2] Institute for Polar Science and Engineering, Jilin University
[3] Polar Research Institute of China

P-13 **Cellulose Nanofibrils Tune the Mechanical, Optical, and Thermal Properties of Ice**
Kiera L. Thompson Towell[1], Olivier Montmayeur[1], Emily Asenath-Smith[1]
[1] Cold Regions Research and Engineering Laboratory (CRREL), US Army Corps of Engineers Engineer Research & Development Center

P-14 **High Pressure Plastic Phases of Water and Water-Ammonia Mixtures**
Maria Rescigno[1,3], Umbertoluca Ranieri[4], Stefan Klotz[2], Sandra Ninet[2], Frédéric Datchi[2], Richard Gaal[3], Livia E. Bove[1,2,3]
[1] Sapienza University
[2] IMPMC
[3] EPFL
[4] University of Edinburgh

P-15 **Ultra-High Vacuum Cryogenic Transmission Electron Microscopy of Ices Indicates the Possible Formation of Hydrogen-Ordered Ices**
Tomoya Yamazaki[1], Akira Kouchi[1], Ken-ichiro Murata[1], Hiroyasu Katsuno[1], Hiroki Nada[2], Tetsuya Hama[3], Yuki Kimura[1]
[1] Institute of Low Temperature Science, Hokkaido University
[2] Faculty of Engineering, Tottori University
[3] Komaba Institute for Science, The University of Tokyo

P-16 **Study of Concentration-Cooling Rate Map of Ice in Aqueous Polymer Solutions by X-Ray Diffraction Measurements**
Yuka Arai[1], Risa Otagiri[1], Kaito Sasaki[2,3], Rio Kita[2,3], Takeru Ito[4], Yoshiki Oda[5], Naoki Shinyashiki[2,3]
[1] Course of Physics, Graduate School of Science, Tokai University
[2] Department of Physics, School of Science, Tokai University
[3] Micro/Nano Technology Center, Tokai University
[4] Department of Chemistry, School of Science, Tokai University
[5] Technology Joint Management Office, Tokai University

P-17 **Pressure Dependence of Dynamics in High-Density Amorphous Ice**
Aigerim Karina[1], Hailong Li[2,3], Tobias Eklund[2,4], Katrin Amann-Winkel[1,2,4]
[1] Department of Physics, Stockholm University, 10691 Stockholm, Sweden
[2] Max Planck Institute for Polymer Research, 55128 Mainz, Germany
[3] Department of Polymer Science & Materials, Dalian University of Technology, Dalian 116024, PR China
[4] Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

P-18 **Structure and Dynamics of Vapor-Deposited Amorphous Ice**
Tobias Eklund[1,2,3], Christina Tonauer[4], Aigerim Karina[5], Hailong Li[2,6], Thomas Loerting[4], Felix Lehmkühler[7], Peter Zalden[3], Katrin Amann-winkel[1,2]
[1] Institute of Physics, Johannes Gutenberg University, Mainz, Germany
[2] Max Planck Institute for Polymer Research, Mainz, Germany
[3] European XFEL, Schenefeld, Germany
[4] Institute of Physical Chemistry, University of Innsbruck, Austria
[5] Department of Physics, Stockholm University, Sweden
[6] School of Chemical Engineering, Dalian University of Technology, China
[7] Deutsches Elektronen-Synchrotron, Hamburg,Germany

P-19 **Temperature and Pressure Effects on the Transformation of Ices**
John S. Tse[1], Robert Bauer[1], Takanori Hattori[2], Shinichi Machida[3], Kazuki Komatsu[4]
[1] Department of Physics and Engineering Physics
[2] Materials and Life Science Division, J-PARC Center
[3] Comprehensive Research Organization for Science and Society (CROSS) Neutron Science and Technology Center
[4] The University of Tokyo

P-20 **Effects of Anti-Freeze Glycoproteins on Long-Term Storage of Cryopreserved Trehalose-Transporter Expressing Cells and on Ice Recrystallization**
Tsutomu Uchida[1], Tsubasa Hohana[1], Sakae Tsuda[2], Takahiro Kikawada[3,4]
[1] Faculty of Engineering, Hokkaido University, N13-W8, Kita-ku, Sapporo 060-8628, Japan
[2] Graduate School of Frontier Sciences, The University of Tokyo, 6-2-3 Kashiwanoha, Kashiwa, 277-0882, Japan
[3] Institute of Agrobiological Sciences, National Agriculture and Food Research Organization, 1-2 Owshi, Tsukuba 305-8634, Japan

[4] Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, 277-8562, Japan

P-21 **Lichen Species Produce Highly Active and Stable Ice Nucleators**

Rosemary Eufemio[1,2], Ingrid de Almeida Ribeiro[3], Todd L. Sformo[4], Gary A. Laursen[5], Valeria Molinero[3], Janine Fröhlich-Nowoisky[6], Mischa Bonn[7], Konrad Meister[1,7]

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[5] High Latitude Mycological Research Institute, University of Montana, Missoula, MT 59801, USA
[6] Max Planck Institute for Chemistry, 55128 Mainz, Germany
[7] Max Planck Institute for Polymer Research, 55128 Mainz, Germany

P-22 **The Role of Antifreeze Proteins in Cellular Membrane Stabilization**

Emily C. Vernon[1,2], Arthur L. DeVries[3], Konrad Meister[1,4]

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[3] Department of Physiology and Biophysics, University of Illinois at Urbana–Champaign, Urbana, Illinois 61801, USA
[4] Max Planck Institute for Polymer Research, 55128 Mainz, Germany

P-23 **Studying the Decisive Factors for Maximum Freezing Efficiency of Bacterial Ice Nucleators**

Galit Renzer[1], Ralph Schwidetzky[1], Mischa Bonn[1], Konrad Meister[1,2]

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[2] Boise State University, 83725 Boise, Idaho, United States

P-24 **Sources of Perchlorate in Antarctic Snow**

Su Jiang[1], Guitao Shi[2], Bo Sun[1]

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[2] East China Normal University

P-25 **Sulfate Concentration and Electrical Conductivity of Firn Cores at Vostok (Central Antarctica) as Proxy of Volcanic Activity over the Past 2,200 Years**

Arina N. Veres[1], Alexey A. Ekaykin[1], Liudmila P. Golobokova[2], Tamara V. Khodzher[2], Olga I. Khuriganowa[2], Alexey V. Turkeev[1]

[1] Arctic and Antarctic Research Institute
[2] Limnological Institute of Siberian Branch of RAS

P-26 **Toward New Impregnation-Refreeze Products for Tomography of Snow Samples?**

Iheb Haffar[1], Frederic Flin[1], Pierre Latil[1], Laurent Pezard[1], Jacques Roulle[1], Pascal Charrier[2], Nicolas Lenoir[2]

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[2] Universite Grenoble Alpes, Grenoble INP, 3SR, CNRS, Grenoble, France

P-27 **Guest Gas-Induced Structural Transformation of Tetra-n-butylammonium Chloride Semi-Clathrates**
Junkyu Lim[1], Joonseop Lee[2], Yongwon Seo[1,3]
[1] Department of Urban and Environmental Engineering, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea
[2] Korea Shipbuilding & Offshore Engineering, Gyeonggi 13591, Republic of Korea
[3] Graduate School of Carbon Neutrality, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea

P-28 **Effect of Functional Group in Dicarboxylate Anions on the Latent Heat Storage Properties of Semiclathrate Hydrates**
Kazuhiro Minamikawa[1], Jin Shimada[1], Takeshi Sugahara[1], Katsuhiko Tsunashima[2], Takayuki Hirai[1]
[1] Graduate School of Engineering Science, Osaka University
[2] Department of Applied Chemistry and Biochemistry, National Institute of Technology, Wakayama College

P-29 **Investigating the Possibility of C_3F_8 as a Gaseous sH Hydrate Former**
Sungwoo Kim[1], Eunae Kim[2], Gyeol Ko[3], Tsutomu Uchida[4], Yongwon Seo[1,5]
[1] Department of Urban and Environmental Engineering, Ulsan National Institute of Science and Technology (UNIST)
[2] Particulate Matter Research Center, Research Institute of Industrial Science & Technology
[3] Korea Shipbuilding & Offshore Engineering
[4] Division of Applied Physics, Hokkaido University
[5] Graduate School of Carbon Neutrality, Ulsan National Institute of Science and Technology (UNIST)

P-30 **Effect of Gas and Water Flow Velocities on Flow Patterns and Gas Uptake of Hydrate Slurries in a Scaled-Up Vertical Plug Flow Reactor**
Ryoka Seki[1], Ryosuke Ezure[1,2], Hiroyuki Komatsu[1], Hideo Tajima[1]
[1] Graduate School of Science and Technology, Niigata University, 2-8050 Ikarashi, Nishi-ku, Niigata 950-2181, Japan
[2] National Institute of Technology, Anan College, 265 Aoki Minobayashi, Anan 774-0017, Japan

P-31 **Raman Spectroscopic Investigation of Clathrates Formation Including C_3F_8 with Various Help Gases**
Tsutomu Uchida[1], Eunae Kim[2], Sungwoo Kim[3], Yongwon Seo[3,4]
[1] Division of Applied Physics, Faculty of Engineering, Hokkaido University, Sapporo 060-8628, Japan
[2] Particulate Matter Research Center, Research Institute of Industrial Science & Technology, Jeollanam-do 57801, Republc of Korea
[3] Department of Urban and Environmental Engineering, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea
[4] Graduate School of Carbon Neutrality, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea

P-32 **Evaluation of Mass Transfer During Clathrate Gas Hydrates Formation by Using Dimensionless Number**
Ryosuke Ezure[1,2], Daiki Nakano[2], Ryoka Seki[2], Hiroyuki Komatsu[2], Hideo Tajima[2]
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[2] Graduate School of Science and Technology, Niigata University, 2-8050 Ikarashi, Niigata 950-2181, Japan

P-33 **Pressure-Induced Phase Transformations and Their Pressure Hystereses of Nitrogen Hydrate**
Ryohei Yonezawa[1], Asa Katsumata[1], Yusuke Yasui[1], Tomoaki Kimura[1], Masafumi Sakata[1], Shigeo Sasaki[1], Takayuki Nagae[2], Ken Niwa[3]
[1] Graduate school of Natural Science and Technology, Gifu University
[2] School of Pharmacy, Tokyo University of Pharmacy and Life Sciences
[3] Graduate School of Engineering, Nagoya University

P-34 **Supercooling Suppression in the Tetrahydrofuran Clathrate Hydrate Formation**
Hironobu Machida[1], Takeshi Sugahara[2], Izumi Hirasawa[3]
[1] Panasonic Corporation
[2] Osaka University
[3] Waseda University

P-35 **Rheological Properties of SF_6 Gas Hydrate Slurry with Surfactant in Horizonal Circular Pipe**
Hideo Tajima[1], Tomoya Sagawa[1], Ryosuke Ezure[1,2], Hiroyuki Komatsu[1]
[1] Guraduate School of Science and Technology, Niigata University
[2] National Institute of Technology, Anan College

P-36 **DFT Calculations of Raman Spectra and NMR Shielding Constants for Large Clusters of Methane Hydrate**
Akira Hori[1]
[1] Faculty of Engineering, Kitami Institute of Technology,

P-37 **Freezing-Induced Acidity Change: Mechanisms and their Possible Impacts on Polar Chemistry**
Radim Štůsek[1]
[1] Department of Chemistry, Faculty of Science, Masaryk University, 62500 Brno, Czech Republic

P-38 **Spectroscopic and Microscopic Study of Freeze-Concentrated Solutions**
Lukáš Veselý[1], Kamila Závacká[2], Radim Štůsek[1], Vilém Neděla[2], Dominik Heger[1]
[1] Department of Chemistry, Faculty of Science, Masaryk University, 625 00 Brno, Czech Republic
[2] Institute of Scientific Instruments of the ASCR, Královopolská 147, 61264 Brno, Czech Republic

P-39 **Exploring the Impact of the Ice Matrix on the Photophysical Behavior of Phenolic Compounds**
Marie Garncarzová[1], Dominik Heger[1]
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Oral Presentations

4-A1-1 13:40-14:20

Physicochemical Processes of OH Radicals on Ice at Low Temperatures

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The physicochemical processes of hydroxyl (OH) radicals on water ice are closely related to various phenomena occurring on ice-dust particles in atmospheric and interstellar environments. Nevertheless, because of intrinsic experimental difficulty in detecting radicals, little is known about the behaviors of radicals on the ice surface. Recently, we have developed the method to monitor the OH radical on ice at very low temperatures, which can open a new phase of research on physicochemical processes of radicals [1]. My presentation will be following two topics.

The behaviors of OH radicals produced by UV-photolysis of H_2O on ice were monitored at temperatures between 54 and 80 K. The OH number density on the surface of ultraviolet-irradiated water ice gradually decreased at temperatures above 60 K. Analyzing the temperature dependence of OH intensities with the Arrhenius equation, we determined the activation energy for surface diffusion for the first time [2].

Recently, we observed experimentally a negative constant current through ice at 10 K when OH radicals coexist with electrons on the ice surface. Using the new method, the surface OH radicals were monitored with and without electrons. We also performed quantum chemical calculations to understand the experimental observations and conclude that once OH adsorbate captures an electron on the surface, the surface OH^- anions trigger the flow of negative current in ice by the sequential proton-hole transfer in ice [3,4]. The OH^- on the surface reproduces H_2O after proton abstraction from neighbouring H_2O. Negative current conductivity was found to be preserved even at temperatures below 50 K, where a positive current by the well-known Grotthuss mechanism is highly suppressed.

1) A. Miyazaki *et al.*, *Phys. Rev. A.* **102**, 052822 (2021).: also see poster by M. Tsuge
2) A. Miyazaki, M. Tsuge, H. Hidaka, Y. Nakai, N. Watanabe, *Astrophys. J. Lett.,* **940**, L2(7pp) (2022).
3) N. Watanabe *et al.*, *Chem Phys. Lett.,* **737**, 136820 (2019).
4) K. Kitajima *et al.*, *J. Phys. Chem. Lett.,* **12**, 704 (2021).

4-A2-1 14:40-15:10

Ice Faces: A molecular view of growth and interactions

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Ice is likely the most ubiquitous solid in the Universe, yet even here on Earth its surfaces contains many mysteries. At atmospheric pressure, the stable form of ice is hexagonal ice I_h with three dominant face: the basal face (familiar as the six-sided shape of snowflakes), the primary prism face (the rectangular sides), and the secondary prism face (a cut across alternate hexagonal apices). This contribution discusses results both from equilibrium-growth and from cutting-edge, nonlinear spectroscopic techniques. Equilibrium growth shows that – contrary to common belief – the stable ice-water interfaces consists of prism and pyramidal faces (diagonal cuts between prism and basal faces) not the expected basal face. A statistical model will be presented that accounts for this result.

There are two hexagonal motifs in the basal face. Electron backscatter diffraction orientation distribution plots correlated with etching images definitively connect one of these to the hexagonal shape of a snowflake answering a question posed by Kepler about 400 years ago. This result has important implications for the molecular level configuration of the prism faces. The surface vibrational spectroscopy sum frequency generation (SFG) shows that the molecular configuration results in unique interactions on each of these faces. SFG results support an ice model consisting of extended, cooperative motion and beyond-bonding-partner determination of hydrogen bond strength. At the molecular level, atmospheric species and aqueous solutes exhibit unique interactions with the faces.

4-A2-2 15:10-15:30

In-Situ Observations of Low- and High-Density Unknown Waters at Interfaces between Water and Ices Grown/Melted by Pressure

Hiromasa Niinomi[1]*, Tomoya Yamazaki[2], Hiroki Nada[3], Tetsuya Hama[4], Akira Kouchi[2], Tomoya Oshikiri[1,5], Masaru Nakagawa[1], Jun Nozawa[6], Junpei T. Okada[6], Satoshi Uda[7], and Yuki Kimura[2]

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Crystallization of ice from water is such abundant phenomena that it governs various phenomena in nature. Hence, it is crucial to understand the non-equilibrium interfacial phenomena between ice and water. Numerical analyses have been performed, providing the widely accepted picture that the order and density of ice continuously change to those of water within a few nm of a transient interfacial layer. However, the actual picture remains unclear because of the lack of experimental investigations. In this presentation, we show, by *in-situ* optical microscopy, that low- and high-density macroscopic unknown water layers separated from bulk water exist at the interface between water and ices (I_h, III and VI) grown/melted by (de)pressure (Fig. 1) [1,2].

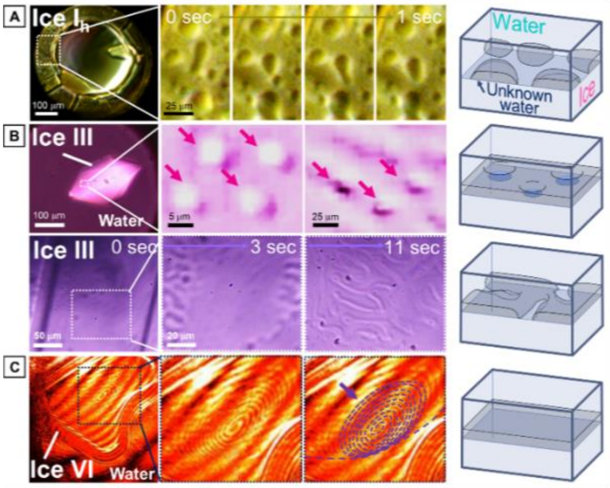

Fig. 1. Micrographs of the *in-situ* observation. Left **A**: Ice I_h, **B**: Ice III, **C**: Ice VI. Right: schematics showing the forms of the unknown waters.

1) H. Niinomi *et al.*, *J. Phys. Chem. Lett.*, **11**, 6779-6784. (2020).
2) H. Niinomi *et al.*, *J. Phys. Chem. Lett.*, **13**, 4251-4256. (2022).

4-A2-3 15:30-15:50

Measurements of negative surface voltage variation of amorphous solid water with a nanoscale spatial resolution by FM-AFM

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Amorphous solid water (ASW) films formed by vapor deposition onto a cold surface are known to have negative surface voltages, which vary depending on the temperature and thickness of the film [1,2]. However, the mechanisms behind the polarization responsible for the surface voltage are still unclear. Previous studies that used Kelvin probe measurements have not provided information on this polarization mechanism because of the lack of spatial resolution. To overcome this limitation in spatial resolution, we used FM-AFM to measure variations in the negative surface voltage of ASW with nanoscale resolution depending on the surface structures.

We conducted measurements on two types of ASW formed by water vapor deposition at 15 and 100K on a Si (111) 7×7 substrate in ultra-high vacuum conditions. The topographic images of the surface structure showed temperature dependence, attributed to the difference in diffusion length of water molecules on the surface until stabilization at the measurement temperature. We also measured variations in the negative surface voltage of ASW depending on the surface structures. In the case of ASW formed at 100K, the negative surface voltage was almost proportional to the height of the surface structure. However, in the case of ASW formed at 15K, the voltages could not be simply scaled to the height of the structure. This implies that the variation in dipole alignment of H_2O, depending on the ice structure, is significant at 15K.

1) M. J. Iedema, M. J. Dresser, D. L. Doering, J. B. Rowland, W. P. Hess, A. A. Tsekouras, J. P. Cowin, *J. Phys. Chem. B*, **102**, 9203-9214 (1998).

2) C. Bu, J. Shi, U. Raut, E. H. Mitchell, R. A. Baragiola, *J. Chem. Phys.*, **142**, 134702 (2015).

4-A3-1 16:10-16:30

Polycrystallinity significantly enhances stress build-up during freezing

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It is well known that when water freezes it can generate large pressures and be very destructive. This is a challenge for many disciplines ranging from civil engineering to cryopreservation [1]. Although freezing damage is commonly attributed to the expansion of water during freezing, experiments suggests that this actually plays only a minor role. In this talk I will show how stresses develop around single and polycrystalline ice crystals, independently of the expansion of water during freezing.

We study the build-up of stresses close to the ice-water interface in an open experimental cell that is coated with a soft elastomer layer [2]. Any stress exerted by the ice crystal leads to a measurable deformation of the elastomer, and thus lets us measure these stresses with high spatial and temporal resolution.

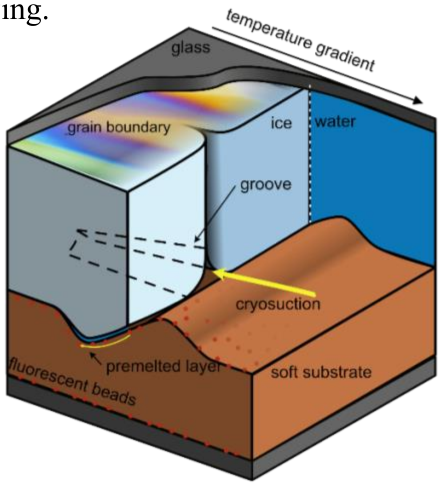

Figure 1: Schematic of a grain boundary groove

We find that polycrystallinity drastically effects the stress build-up dynamics. Small, liquid filled channels (grain-boundary grooves) at the intersection of ice grain boundaries act as supplies of water that feed ice growth and associated stress build up at localised positions over the ice surface. This new ice growth has a high propensity for damage. Interestingly, the dynamics of the process is hard to predict accurately. Our insights shed light on some of the difficulties involved in making accurate models for freezing porous materials.

1) J.G. Dash, A.W. Rempel, and J.S. Wettlaufer, *Reviews of Modern Physics* 78, no. 3 695–741 (2006)
2) D. Gerber, L. A. Wilen, F. Poydenot, E. R. Dufresne, and R. W. Style, *Proceedings of the National Academy of Sciences* 119, no. 31 (August 2022)

Growth and Form of Rippled Icicles

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[2]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, Amsterdam 1098XH, Netherlands

Icicles are known for their universal conelike shape and rippled surface, and for both these features theories have been developed. However, experimental results appear to be at odds with the existing theories: for pure water in fact very irregular icicles are observed, and it is only if some salt is present that the cone shape and the surface ripples are observed. Here, we investigate the effect of such impurities on the morphology of icicles. We observe surface ripples with a wavelength of approximately equal to 1 cm that is independent of impurity concentration. Surprisingly, the amplitude of the ripples is zero for ultrapure water and increases rather sharply with impurity concentration.

We find that the expulsion of salt from the ice crystal leads to a transition between partial to complete wetting of the water on the icicle, and it is only for the latter case that the icicles become well behaved. This is confirmed by adding a small amount of dye to the water that has different color in the liquid and solid phase, and image the growing icicles. These experiments show that in the presence of impurities in the water (causing complete wetting), the icicles are covered with a thin liquid film that speeds up icicle and ripple growth. In contrast, icicles grown from ultrapure water exhibit partial wetting, and grow due to droplets sliding down in stick-slip motion, leading to an ill-defined overall shape that differs from the theoretically predicted one, and a disappearance of the ripples.

Demmenie, M., Reus, L., Kolpakov, P., Woutersen, S., Bonn, D., & Shahidzadeh, N. Growth and Form of Rippled Icicles. *Physical Review Applied*, *19*(2), 024005 (2023).

With Nature highlight:
https://www.nature.com/articles/d41586-023-00350-4

Ice Removal from Surfaces by Interfacial Crack Propagation

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The study of ice adhesion is more complicated than just measuring the force required to remove the ice from a surface of interest. There are many diverse scenarios under which ice forms and these various forms of ice adhere to and delaminate from surfaces differently. Ultimately, the key issue in the field of ice adhesion is that there are no formal standards for assessing the ice mitigation potential of (passive) surface coatings [1] and physics-based analysis approaches are lacking. As a result, there are almost as many ice adhesion tests across the field as there are researchers developing coating technologies to passively mitigate icing.

The focus of this talk is on research about testing methods and analysis approaches for ice adhesion. The growth/adherence of ice on/to surfaces will be discussed, including methods to achieve control over ice microstructure at variable temperatures using crystallization from the melt apparatus [2]. Ice adhesion testing configurations will be addressed, including shear and tensile delamination modes [3]. Being able to test the ice adhesion properties of materials using different ice types, delamination modes, and sizes, using a single geometry, is a promising approach to the development of analysis methods for ice adhesion data. Experimental results on ice adhesion testing and surface characterization will be presented along with a structural mechanical computational model to provide insights into generalizable analysis methods.

1) K.L Mittal, C.-H Choi, “Ice Adhesion: Mechanism, Measurement, and Mitigation,” Scrivener Publishing, Beverly, MA, (2020).
2) E. Asenath-Smith, G.R. Hoch, C.T. Erb, *J. Cryst. Growth*, **535** (2020) 125563.
3) A.R. Lovell, G.R. Hoch, C.J Donnelly, J.M. Hodge, R.B. Haehnel, E. Asenath-Smith, *ERDC/CRREL Tech. Report*, **TN-21-1**, 1 (2021).

4-A4-1 17:30-17:50

Hydrogen bonding in water enhanced by local electric field in polyelectrolyte brushes

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A polymer electrolyte brush is a reasonable platform to confine water molecules within a nanoscopic area to study their role in the function of interacting media because of their adjustable nanospace and charge by changing the in-plane density and side chains of the brush. Here, we demonstrate how the in-plane spacing of cationic polymer brush chains, poly[2-(methacryloyloxy)ethyltrimethylammonium chloride] (PMTAC), affects the hydrogen bond configuration of incorporated water using soft X-ray emission spectroscopy [1]. At the critical in-plane density $\sigma = 0.30$ chains/nm^2 of PMTAC, tetrahedrally coordinated (ice-like) water molecules started to melt into distorted or broken hydrogen-bonded configurations. Considering the charge on the quaternary ammonium cations, the electric field required to form a tetrahedrally coordinated hydrogen-bonded configuration was estimated as ~500 kV cm^{-1} and is effective up to ~ 1 nm from the surface of the polymer chain [2].

1) K. Yamazoe, Y. Higaki, Y. Inutsuka, J. Miyawaki, A. Takahara, Y. Harada: *Langmuir*, **38**, 3076 (2022).
2) Z. He, W. J. Xie, Z. Liu, G. Liu, Z. Wang, Y. Q. Gao, J. Wang, *Sci. Adv.*, **2**, e1600345 (2016).

Adsorption Structures of Ammonia Molecules on Crystalline Ice

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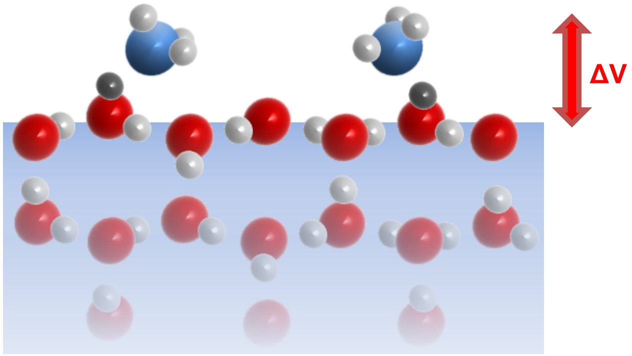
The interactions between adsorbed molecules and an ice surface are strongly influenced by the ice surface, which contains dangling H atoms and O atoms. In this study, we studied the ammonia molecules adsorbed on the basal surface of crystalline ice (CI). The adsorption structure of ammonia was examined using various experimental techniques such as temperature programmed desorption, low energy sputtering, reflection-absorption infrared spectroscopy, and surface voltage measurements. At low ammonia coverages on ice, the ammonia molecules adsorbed exclusively on the dangling H sites of the ice surface through the formation of N···H−O bonds. Additionally, the ammonia molecules were tilted towards the surface. Once the dangling H sites became saturated, further-adsorbed ammonia molecules form a multilayer with isotropic orientation. To measure the surface density of free O−H groups, we conducted a titration experiment, and it showed the density is 0.29 ± 0.04 monolayers, indicating the basal surface of CI is not reconstructed notably.



1) D. H. Lee, H. Kang, *J. Phys. Chem. C,* **127,** 2885–2893 (2023)

4-B2-1 14:40-15:10

Measuring microscale mechanisms of snow melt, rain-on-snow, drainage, and imbibition using rapid magnetic resonance profiling.

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The effective hydraulic conductivity of snow is highly impacted by dynamic microstructures and time dependent phase changes at the pore scale, yet these mechanisms have never been investigated at the pore scale. This inhibits improvements on the constitutive laws for larger scale models of snow hydrology using upscaling methods. We bridge this gap by using rapid profiling of liquid water content in snow with nuclear magnetic resonance methods at a resolution of 100 micron and 50 ms. The data shows that we can clearly measure saturation profiles and velocity fluctuations during snow melt and rain on snow events in a laboratory setting. We observe the transition from matrix flow to preferential flow in snow as well as compaction in wetted porous media. We compared the data to a model media consisting of sticky-glass beads of 1 mm. These media are static and do not experience pre-wetting and phase transitions. As a result, we observe that wetting fronts and drainage processes can migrate an order of magnitude faster in snow than in static model media with similar grainsizes. This is the first time that wet snow metamorphism such as compaction of wet snow and collapses of weak layers can be observed in real time at a resolution that reveals flow and phase-change processes at the microscale. This methodology has the potential to answer many open questions in wet-snow mechanics such as the onset of wet-snow avalanches and can be applied much broader in sea-ice metamorphism and multi-phase flow in porous media.

4-B2-2 15:10-15:30

Ice particles in clouds: origins, processing, and cloud lifetime.

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Mixed-phase clouds are characterized by the inherently unstable co-existence of ice and liquid water and are especially important for the Earth's energy budget and precipitation processes. In general, clouds can have either a warming or cooling effect on the Earth's surface, but the balance is sensitive to cloud type, amount, and microphysical state. At times mixed-phase clouds can persist for days and their persistence is the result of a sensitive balance between moisture availability, precipitation, sublimation, and the supply of aerosol particles that act as the cloud seeds. Particles that catalyze the formation of atmospheric ice (ice nucleating particles, INP) are of particular interest because they are a small subset of the atmospheric aerosol and their abundance is often seemingly disconnected from cloud properties, like cloud ice or precipitation. Here I discuss a range of INP investigations that are aimed at understanding how the nucleation and evolution of cloud ice ultimately affects cloud phase and lifetime [1,2]. The potential for human emissions to the atmosphere to influence cloud properties are discussed.

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4-B2-3 15:30-15:50

Direct Observation of Wet Snow Using X-ray Tomography: First Results and Outlooks

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For more than 20 years, X-ray microtomography (μCT) has been extensively used to study dry snow (see e.g. [1, 2]). However, imaging of wet snow still resists the μCT approach for several reasons: (1) the low absorption contrast between ice and liquid water, (2) the difficult temperature regulation at 0 °C and (3) some very rapid processes that may occur during ice melting and water percolation. Despite multiple attempts to provide tomographic images of wet snow, the literature studies only report refrozen states [3, 4] or indirect evaluations by difference imaging.

We recently carried out several experiments that solved most of the problems mentioned above: using a specifically modified version of our cold stage CellStat [5], we were able to obtain relatively well thermalized samples at 0 °C, allowing to stabilize the ice-water interfaces for μCT acquisitions. A low energy approach using the 3SR laboratory tomograph was first used to provide snow images where the evolution of air, ice and liquid water can be detected at a voxel size of 5 to 8 μm. More recently, synchrotron tomography at Anatomix beamline provided much higher quality image series at the resolution of 3 μm using phase contrast tomography, which opens new outlooks for the study of wet snow.

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Pattern Formation of Refrozen Melt Structures in Snowpack

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Infiltration of surface-generated meltwater into snowpack is a spatially heterogeneous process due to a gravity fingering instability that is intrinsic to unsaturated flow in porous media. Upon contact with deeper and colder firn, such melt may refreeze into existing porous structures during infiltration. As a result of the coupling between gravity fingering and the water/ice phase transition, refrozen meltwater forms as one of two primary structures within preexisting snowpack: (1) horizontal frozen structures that act as a barrier for infiltration (ice lenses or ice sheets) and (2) vertical frozen structures (ice pipes) which may facilitate deeper meltwater infiltration. These two classes of refrozen structures have been observed in the field and have profound effects on how meltwater and its residual thermal content distributes into the snowpack [1]. However, a more detailed physics-based understanding of these structures has not yet been posed.

In this work, we use the thermodynamic nonequilibrium meltwater infiltration model developed by Moure et al. [2] to investigate the formation of refrozen melt structures within an initially homogeneous snowpack. The model is able to account for various hydraulic properties and initial thermal conditions of the snowpack, as well as a time-varying rate of meltwater influx. As the temperatures of the ice and water phases are tracked independently, the refreezing kinetics of infiltrated meltwater are governed by local thermodynamic conditions of each phase and thus do not rely on the assumption of a constant rate of freezing. By performing extensive numerical simulations of the model, we are able to recover the formation of ice lenses and ice pipes across a broad range of snowpack parameters. We identify the key thermal conditions that lead to the formation of these structures and how they continue to evolve in time under changing climatic conditions.

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4-B3-2 16:30-16:50

A Physical Model of Gas Bubble Nucleation and Transport in Sea Ice

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Sea ice forms when saline ocean water freezes. This ice has a porous structure of solid ice and liquid brine. Freezing concentrates dissolved gas species present in ocean water, which can subsequently exceed saturation and nucleate as bubbles. These gas bubbles can rise under their own buoyancy and escape to the atmosphere, or redissolve into the liquid inclusions. The resulting transport is a key physical uncertainty for the flux of climatically important gases between the ice and the atmosphere, as well as the biogeochemical and optical properties of the ice.

We develop a phenomenological model for the motion of a bubble rising in porous sea ice which includes viscous drag and bubble trapping. We apply this description of bubble transport in a 3-phase thermodynamic model of the growth of porous sea ice, comprising of a solid ice matrix filled with liquid brine and gas bubbles. Our model extends the traditional mushy-layer theory describing the solidification of saltwater solutions to include a gas phase. The resulting model is solved numerically to investigate gas dynamics during a seasonal cycle of ice growth and melt. We find that the total gas flux to the atmosphere during a season is highly sensitive to the ratio of the bubble size to the characteristic scale of the ice pore geometry.

4-B3-3 16:50-17:10

Effects of Sulfuric Acid on Sintering of Laboratory Simulated Polar Firn

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It has been well-documented that soluble impurities exist within the ice and snow of the Earth's polar regions. However, the role of these impurities in the mechanical strength, densification, stratification, and rheology of ice and firn remains poorly understood. To address this knowledge gap, from within a controlled cold-laboratory environment, we have conducted a series of snow grain sintering experiments to investigate the effects of sulfuric acid (H_2SO_4) on simulated samples of polar firn. H_2SO_4 is naturally produced in the Earth's atmosphere, before being deposited back on Earth's surface via precipitation events. To study its potential effects on the bonding and metamorphism of individual snow grains, we conducted a series of experiments to observe how trace amounts of H_2SO_4 (~50ppm) may or may not influence both the long-term sintering and sub-second sintering processes of simulated samples of polar firn and loose snow. We then compared our results to a parallel set of experiments conducted with de-ionized water to serve as a control test set. To analyze sub-second sintering processes, angle of repose experiments were completed at -5, -10, -15, -20, -25, and -30°C. Simultaneously, a 256-day experiment was also conducted where a time-series of micro-computed X-Ray Tomography (micro-CT) data was collected while maintaining samples at an isothermal temperature of -3°C. In our results, we found that the addition of H2SO4 in ice grains resulted in higher angles of repose at temperatures above -15°C, suggesting a direct effect on sub-second sintering processes at relatively warm temperatures, while below -15°C there was no discernible difference in the angles of repose. Additionally, unconfined uniaxial compression tests were completed on two systems; a materials testing stage (MTS) that fits within the confines of an x-ray computed micro-tomography chamber and an *MTS Systems* Criterion 43 MTS with a liquid nitrogen-cooled environmental chamber. Tests were conducted at temperatures between -5 and -30°C and displacement rates between $1*10^{-4}$ and $1*10^{-5}s^{-1}$. Results from both compression testing instruments revealed an enhanced ductility of the H_2SO_4 doped specimens.

Investigation of structure and geochemical composition of Ushkovsky shallow ice core

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The glacier ice cores are excellent archive that contain various data of climate of the past. They allow to create long-term paleoclimatic reconstruction with high resolution (up to seasonal variation).

Many works are devoted to such reconstructions for different Earth regions. But for the northeast Asia there are a few based on ice core drilled at Ushkovsky ice cap (altitude, 3903 m), Kamchatka, Russia in 1998 [1].

Here we present for the first-time data on the chemical (Na^+, NH_4^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, NO_3^- , SO_4^{2-}) and isotope (δ18O and δD) composition and stratigraphic analysis of a shallow ice core (14 m) also drilled at Ushkovsky ice cap (altitude, 3900 m), Kamchatka, Russia in 2022. These results can complement the previous one obtained from the first Ushkovsky ice core.

Seasonal variation of values is observed for NH_4^+ and d-excess. For dating correction, we use tephra analysis combined with chemical composition. According to which we make an attempt to reconstruct the dynamic of sea ice, forest bioproductivity and wildfires in the Kamchatka region.

Supported by grant of RSF-22-17-00159

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4-B4-2 17:50-18:10

Mechanism Research on Ice Core Adaptively Breaking For A New Ice-drilling Method of Continuously Coring with Air Reverse Circulation

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In recent years, a new ice-drilling method of Continuously Coring with Air Reverse Circulation (CCARC) with a rapid-air-movement (RAM) ice drill system has been put forward (the scheme of this method is shown in Figure 1), which uses dual-wall aluminum drill pipe. CCARC ice drilling technology can effectively prevent compressed air circulation losses in snow-firn cover and it can continuously get ice core with air reverse circulation. It does not need to stop drilling to lift the drill to the ice-sheet surface to take out ice core from the drill, so it can greatly improve the rate of penetration (ROP). However, the prerequisite for the realization of CCARC ice drilling is that the core splitter set on the internal surface of the inner tube of drill bit can adaptively break ice core with equal length. In order to further improve CCARC ice drilling technology, it is necessary to study horizontal force and lateral displacement required to break ice core with different diameter and length during drilling, because these key parameters are important for ice coring drilling operation and drill design. Thus, in this study, based on the established ice-core splitting test-bed, mechanism and key parameters of ice-core breaking process under different conditions were theoretically calculated and experimentally measured. Then the influence of ice core temperature, diameter and splitting length on ice core breaking were quantified, and the feasibility of the ice-core breaking mode was also demonstrated.

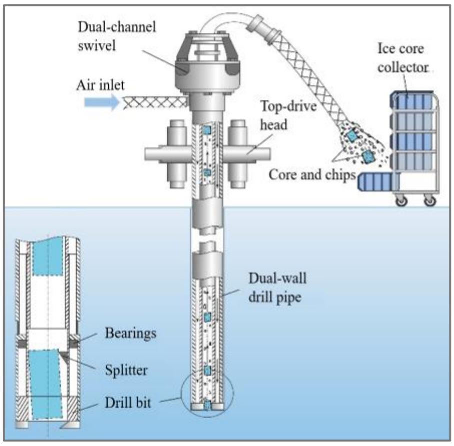

Fig. 1 The schematic diagram of ice core continuously coring with air reverse circulation

4-B4-3 18:10-18:30

International efforts and Chinese contributions on mapping subglacial topography of the Antarctica Ice Sheet

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Poor knowledge on subglacial conditions and processes leads directly to “deep uncertainty “in evaluating and predicting the instability of the Antarctic Ice Sheet (AIS), which could cause catastrophic rising of sea level. Subglacial topography of the AIS is the main control of subglacial conditions and processes, and is also a precondition to understand the Antarctica.

In the past seven decades, based on extensive international collaborations, subglacial topography of the AIS has been continuously detected through airborne IPR. Digital elevation models of subglacial topography, like Bedmap, Bedmap 2 and the upcoming Bedmap 3, have been compiled successively. Since 2004, China has made significant progresses on grounded and airborne platform configuration, IPR development, field surveying and data processing method. So far, China has become an important contributor to international efforts on mapping subglacial topography of the AIS, and is playing an important role in the SCAR Bedmap 3 project.

Freezing damage in brittle hydrogels

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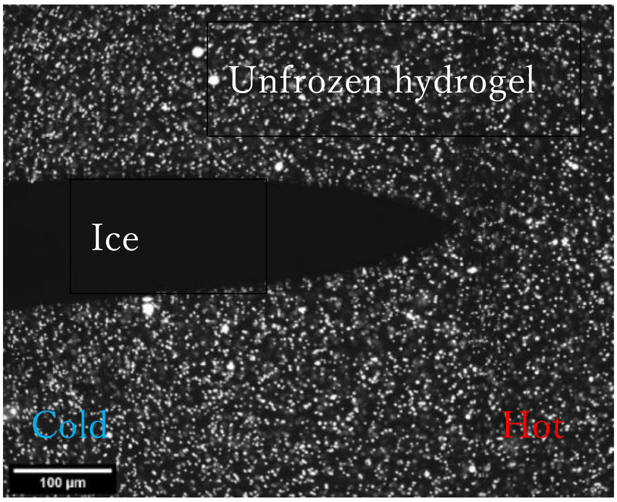
We study how freezing breaks soft, porous materials by freezing model hydrogels, while imaging the sample with a confocal microscope (e.g. [1]). This technique allows us to reconstruct the ice's 3D shape as it breaks the hydrogel open, as well as the stresses and strains that occur in the hydrogel. The ice shape looks just like a crack that we might expect if we simply tore the hydrogel apart (see the Figure). Indeed, we directly connect the macroscopic material properties of the hydrogel (e.g. stiffness and fracture toughness) to how the hydrogel fails during freezing. Further, we reveal the critical conditions at which the hydrogel will break. Our work helps us understand how damage arises in more complex soft materials like soils and biological tissue.



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Step-bunching instability of growing interfaces between ice and supercooled water

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Ice-crystal growth in supercooled water is one of the most familiar examples of phase-transition dynamics, playing essential roles in various natural phenomena on Earth. Despite its fundamental importance, the microscopic view at the elementary step level remains elusive. Here, using an advanced optical microscope, we find self-organization of elementary steps during ice-crystal growth, called step-bunching instability (SBI), driven by the competition between step dynamics, interfacial stiffness, and latent heat diffusions [1]. Although the SBI itself has been observed in a broad range of crystalline materials, there has been no firm experimental proof of the SBI for simple melt growth so far.

We made direct visualizations of spatiotemporal dynamics of the SBI during the growth of ice and the spontaneous formation of the spiral growth induced by the SBI. In addition, using a two-beam interferometer, we directly measured not only the characteristic step spacing and the step-advancing velocity, but also the height of the bunched steps. This quantitative in-situ approach allows us to elucidate the underlying mechanism of this SBI at the level of interactions between elementary steps. Our finding offers a significant clue to understanding the general mechanism of melt growth beyond ice-crystal growth, inseparably involving several broad research fields, including cryobiological, geophysical, and material branches.

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5-A1-2 9:30-9:50

Liquid-Cell Transmission Electron Microscopy of ice crystals and bubble behaviors in the ice

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Transmission electron microscopes can observe materials with high temporal and spatial resolution. However, it is necessary to use special techniques to observe volatile samples, such as water, because it requires a high vacuum environment. Such volatile samples can be observed by liquid-cell transmission electron microscopy (LC-TEM), which these samples were sandwiched between two electron transparent thin films to isolate the high vacuum environment and the liquid sample [1]. Because this method allows us to perform in situ observation of liquid samples by TEM, crystal nucleation events from aqueous solutions have been captured and the nucleation processes have been investigated [2,3]. In addition, we developed a cooling TEM specimen holder using Peltier devices that can maintain a specimen at temperatures ranging from room temperature to minus several tens of degrees Celsius, which is difficult to keep at that temperature using refrigerant such as liquid nitrogen. Now we combine this holder with liquid cell to establish the system that can observe liquid specimens to be cooled to minus several tens of degrees Celsius. This system is expected to be used to observe phenomena involving water and ice, such as the formation of ice crystals from water and surface melting, which have been difficult to access with previous electron microscopic techniques.

In this study, we will report first that we succeeded in observing ice crystals with this system. We will also report that the observation results about bubbles formed in the ice and their behaviors near the ice surface.

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5-A1-3 9:50-10:10

Characterizing Faceted Snow Crystals with Electron Backscatter Diffraction

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Electron Backscatter Diffraction (EBSD) in the cryosphere has been primarily used to characterize the crystallographic orientation of ice, primarily glacial and sea ice. However, to our knowledge, EBSD has not yet been successfully applied to snow, given that successful EBSD mapping requires both parallel and polished surfaces and samples that can be tilted to 70° beyond horizontal without rotation or translation of the medium. Moreover, the data obtained from EBSD is imperative to better understand grain growth kinetics, mechanical response, and radiative transfer properties of snow as it relates to the fabric evolution of seasonal or polar snow. Here we present a methodology to obtain successful EBSD indexing and mapping of faceted snow crystals (depth hoar and surface hoar) collected from the field and grown within a controlled cold-laboratory environment. Central to this method, is casting the snow samples with dimethyl phthalate before using a biological sledge microtome to obtain parallel planed and smooth surfaces. In our results, we show that EBSD indexing could be completed successfully on hexagonal and rectangular depth hoar crystals using this method, and further that the growth of the depth hoar crystals occurred primarily along the basal plane for hexagonal cups and along both the primary and secondary prismatic planes for rectangular-shaped cups. Additionally, EBSD of single grains of casted surface hoar showed that crystal growth had occurred primarily along the primary prismatic plane. Given the success of our newly developed method for performing EBSD on snow crystals, we are hopeful that it will act to complement other established or developing techniques for elucidating snow crystal orientation, such as the Automatic Texture Analyzer for c-axis orientations and Diffraction Contrast Tomography for c- and a-axis orientations, respectively.

5-A2-1 10:30-10:50

Microscopic ordering of supercooled water on the ice basal face

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Growth of ice crystals from supercooled liquid water (the melt growth of ice) exhibits anisotropic kinetics depending on the nature of the exposed ice surface, in which the basal face is known to grow much slower than the prism and secondary prism faces [1, 2]. The underlying anisotropy in molecular attachment and its link to the interfacial structure has been of great interest in fundamental sciences [3] as well as various applications in sub-zero environments, e.g., the recognition of different ice surfaces by anti-freeze proteins and the resulting molecular insights for cryopreservation [4]. However, despite intensive studies due to its broad significance, the microscopic mechanism resulting in the anisotropic growth kinetics remains elusive.

To elucidate its origin, using extensive molecular dynamics simulations, we comprehensively explore how supercooled water molecules are incorporated into the ice basal face [5]. Structural and dynamic characterizations of the ice-water interface demonstrate that the ice basal face is sharp at the molecular level and its growth proceeds layer-by-layer through two-dimensional nucleation without any intermediate structures. We further quantify the crossover from layerwise to adhesive growth, called kinetic roughening, with the height difference correlation and the normal growth rate analysis. Moreover, we identify the presence of an ultra-low density water layer in contact with the structural interface, which assists two-dimensional nucleation at a small amount of supercooling without involving any triggers, such as dislocations.

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5-A2-2 10:50-11:10

Effect of Air Molecules on the Growth Kinetics of Ice from Water Studied by Molecular Dynamics Simulation

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The molecular-scale growth kinetics of ice from water in the presence of air molecules are still poorly understood, despite their importance for understanding ice particle formation in nature. In this study, a molecular dynamics simulation is conducted to elucidate the molecular-scale growth kinetics at the interface between a (111) plane of cubic ice and water in the presence of N_2 molecules.1) N_2 molecules bind stably to the interface for a period of 1 ns or longer. Free-energy surfaces of an N_2 molecule along the interface and along an ideal (111) plane surface of cubic ice suggest that for both models, the position where an N_2 molecule binds stably is different at the interface and on the ideal plane surface, and the stability of the binding is much higher for the interface than for the ideal plane surface. Stacking-disordered ice grows at the interface, and the formation probability of a hexagonal ice layer in the stacking-disordered ice is higher for the charged model than for the uncharged model. The formation probability for the hexagonal ice layer in the stacking-disordered ice depends not only on the stability of binding but also on the positions where N_2 molecules bind on the underlying ice, and the number of N_2 molecules that bind stably to the underlying ice. At the presentation, we will also discuss the growth kinetics at the interface for (0001) basal, (10 -10) prismatic and (11 -20) secondary prismatic planes of hexagonal ice in the presence of N_2 or CO_2 molecules.

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5-A2-3 11:10-11:30

Toward the Rational Design of Novel Cryoprotectants

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Emerging medical treatments such as cell-based therapies rely on our ability to cryopreserve (i.e. to freeze and then thaw) biological material for storage or transport – without damaging it in the process [1]. To control the formation of ice in this context we use cryoprotectants. These are molecules that (amongst other things) manage to curb ice re-crystallization, i.e., the uncontrolled growth of large ice crystals – one of the main causes of cellular damage. However, the current cryoprotectants are far from being ideal – they are costly, toxic, and not especially effective. To make things worse, we have been using the very same cryoprotectants for the past 50 years, as the search for new and better ones has largely been a trial-and-error exercise. Why? Because *"the molecular mechanisms underlying these processes remain largely unknown"* [2] .

Here, we brought together experiments and simulations to tackle the long-standing, fundamental question of how exactly different molecules interact with growing ice crystals and succeed (or not!) in preventing ice re-crystallization.

To do so, in the past few years we investigated the interfaces between ice and polymers [3], peptides [4] and amino acids [5]. However, it became clear that each class of molecules has its own story to tell when it comes to inhibit ice re-crystallization. Thus, we have recently developed a machine learning model, based on descriptors obtained via molecular dynamics simulations, to understand and ultimately predict the ability of a given molecular specie to limit ice re-crystallization. As a result, we are now paving the way towards the rational design of the next generation of cryoprotectants.

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5-A2-4 11:30-11:50

A self-oscillatory growth model of an ice crystal in antifreeze glycoprotein solution

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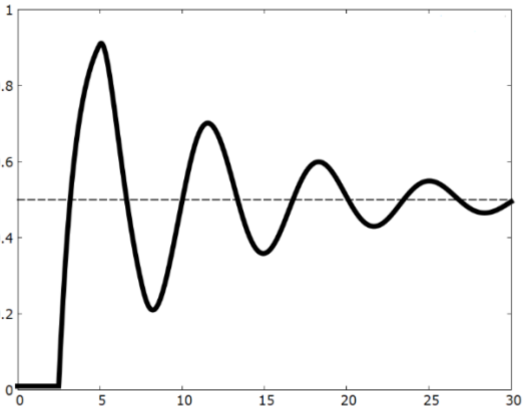
The oscillatory growth of ice crystals in supercooled water including an impurity of antifreeze glycoprotein (AFGP) molecules has been observed under microgravity conditions on the International Space Station [1]. The interfacial adsorption of AFGP molecules on ice can make the oscillation of the growth rates. In this study, we propose the new model taking account of a time delay of adsorption to explain the formation of self-oscillatory growth of an ice crystal without a change of external conditions.

We consider a dimensionless time dependent Langmuir adsorption equation including the delay $T > 0$, in which the uncovered area of ice interface by impurity depends on the number of AFGP impurity molecules n at a time $t - T$, not at t. This means the conformational change of an AFGP molecule takes the time T during its adsorption process. The Figure 1 shows the damping oscillation of $n(t)$ for $T = 2.5$ and $n(0) = 0.01$. If the growth rate $V(t)$ of ice crystal is a function with respect to $n(t)$, the oscillatory behavior of $V(t)$ occurs. We found the oscillation period of $n(t)$ is a few times T, that is, the period increases with T. The detail discussion will be in the presentation.

Figure 1 dimensionless $n(t)$



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Surface phase transitions, anomalous step free energies and crystal growth rates of ice in the atmosphere

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As temperature is cooled down, ice crystals in the atmosphere change their habit from plates, to columns, to plates and back to columns in a puzzling sequence first reported by Nakaya almost 75 years ago [1]. However, the underlying physics of this enigmatic behavior has remained unexplained.

In this work we exploit a methodology for the study of surface fluctuations developed in the last years in our lab to unveil the structure and dynamics of the ice surface [2,3,4]. We show that in the range from -80 to 0 ºC, the main crystal facets of ice undergo a sequence of alternating structural surface phase transitions that result in the anomalous increase of step free energies and the crossover of crystal growth rates exactly as required to explain Nakaya's experimental observations [3]. Our results emphasize the significance of the equilibrium surface structure as the essential feature governing widely different phenomenon of ice physics ranging from the growth rates of ice crystals in the atmosphere, to the low friction coefficient of snow [4,5].

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5-A3-2 13:50-14:10

Temperature Dependence of the Growth Kinetics of Elementary Spiral Steps on Ice Prism Faces Grown in Vapor

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To understand the growth kinetics of ice crystals at the molecular level, we need to measure the kinetics of the lateral growth of individual elementary steps. To achieve such measurements, we have so far developed advanced optical microscopy (named LCM-DIM), which can visualize elementary steps (0.4 nm in thickness) on ice crystal surfaces [1]. By LCM-DIM, we systematically studied the growth kinetics of elementary spiral steps on ice basal faces that were heteroepitaxially grown on a cleaved AgI crystal [2,3].

In contrast, studies on a prism face (another important facet of an ice crystal) are still very preliminary because of the lack of such heteroepitaxial substrate. Therefore, in this study [4], we first tried to find a heteroepitaxial substrate and found that a prism face of a CdSe crystal can work as a heteroepitaxial substrate for ice prism faces.

Then we observed the lateral growth of elementary spiral steps on ice prism faces in vapor. On prism faces, we found that outcrops of screw dislocations are mostly located in the interiors of prism faces and that distance L between adjacent spiral steps is uniform, whereas these two features are not observed on basal faces. From the supersaturation dependence of the lateral velocity V_{step} of elementary spiral steps, we determined the step kinetic coefficient β on prism faces in a temperature (T) range from −25.0 to −2.6 °C and found that β on prism faces decreases monotonically with decreasing T (ordinary Arrhenius-type behavior). In contrast, from the relation between L and the driving force for the crystallization $\Delta\mu$, we found that the step ledge free energy κ on prism faces presents an extraordinary peak at T~-15°C, implying the change in surface structure at this T. The T dependences of β and κ measured on prism faces [4] are significantly different from those on basal faces [3]. To elucidate the reasons for these differences, we need to study T dependence of surface structures of prism faces in the future.

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5-A3-3 14:10-14:30

Uptake Mechanism of Atmospheric-Concentration HCl Gas in Ice Crystals via Hydrochloric Acid Droplets

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Surfaces of ice act as sites of various chemical reactions of atmospheric acidic gases, which cause serious environmental issues, such as the catalytic ozone depletion by hydrogen chloride (HCl) gas. However, the reported amounts of the uptake of HCl by ice surfaces exhibited considerable variations. One of the plausible causes for the variations is the presence/absence of quasi-liquid layers (QLLs) on ice crystal surfaces. Hence, we performed direct observations of ice basal faces under atmospheric-concentration HCl gas (~10-4 Pa) [1] by laser confocal microscopy combined with differential interference contrast microscopy (LCM-DIM), which can directly visualize 0.37-nm-thick elementary steps and QLLs on ice crystal surfaces [2].

Even in the presence of HCl gas, we found that liquid droplets appeared on ice basal faces at temperatures lower than -10 °C. However, the droplets were not pure water but an HCl aqueous solution, whose HCl concentration was the same as those of a liquidus line of a binary phase diagram of water and HCl. The lateral advancement of the elementary step was pinned by the HCl droplets, resulting in the formation of bunched steps. Eventually, by the lateral growth of the bunched steps, which had enough height, the HCl droplets were embedded in the ice crystal (Fig. 1). These results indicate that a bulk of an ice crystal plays an important role in the uptake of HCl.

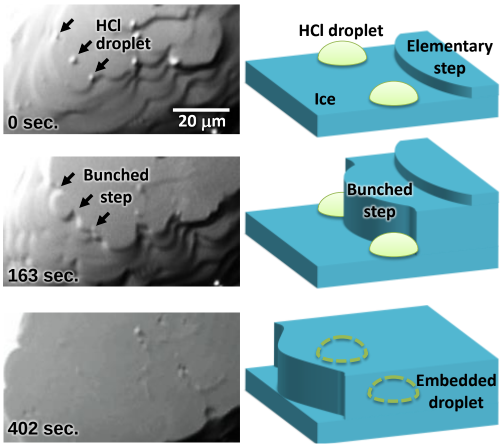

Fig. 1 HCl droplets embedded by the bunched steps of ice.

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5-A3-4 14:30-14:50

Quantification of Anion and Cation Uptake in Ice Ih Crystals

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Small amounts of ions are incorporated into ice crystals and could have direct impact on desalination processes, climate change and further understanding of icy satellites. These small ion dopants can alter the fundamental physical and chemical properties of ice, such as the structure and electrical conductivity. Here we examine the influence of the uptake of three environmentally relevant salts, ammonium chloride, sodium chloride, and ammonium sulfate, in ice *Ih* formation using capillary electrophoresis (CE). By using both cation and anion modes, we observed and quantified the uptake of individual ions into the ice. Our results indicate that anions have a higher propensity for inclusion into ice Ih crystals. [1]

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5-A3-5 14:50-15:10

Solute Interactions in Ice: Color Quenching and Crystallization Effects

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We have observed that some conjugated solute molecules lose color upon entrapment in ice and may affect crystallization phenomena. The shape of ice crystals depends greatly on kinetic factors in the crystallization micro-environment. For example, anti-freeze proteins have a well-documented ability to shape ice crystals by adsorption to growth planes, thereby inhibiting rampant growth in biological systems [1]. Similarly, a molecular solute was reported to modulate ice crystallization via supramolecular assembly to enable binding to ice surfaces during growth [2]. Widely, ice crystallization studies are focused on how molecular solutes and additives modify ice growth. Research that considers how the properties of molecular species are modified by entrapment within the ice microstructure are far less common.

The color quenching characteristic of dyes when frozen is a novel phenomenon in the field of ice crystallization, and we have used both experimental and computational studies to investigate the interactions between ice and solutes. Experimental studies with UV-Vis spectroscopy and fluorescence microscopy show that color quenching depends on pH and does not depend on ice microstructure. Ice crystallization studies indicates that the solutes can modify crystal habit depending on concentration. Density functional theory and molecular dynamics studies were used to study the role that hydrogen bonding, orientation of solutes at ice surfaces, and intramolecular interactions play in the observed color of solute frozen in an ice matrix.

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5-A4-1 15:30-16:00

Ultrafst Melting and Recrystallization Dynamics of Ice Revealed by Time-Resolved X-ray Scattering at FELs

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The phase transition between water and ice is ubiquitous and one of the most important phenomena in nature. Here, we performed time-resolved x-ray scattering experiments capturing the melting and recrystallization dynamics of ice. The ultrafast heating of ice I is induced by an IR laser pulse and probed with an intense x-ray pulse, which provided us with direct structural information on different length scales. From the wide-angle x-ray scattering (WAXS) patterns, the molten fraction, as well as the corresponding temperature at each delay, were determined. The small-angle x-ray scattering (SAXS) patterns, together with the information extracted from the WAXS analysis, provided the time-dependent change of the size and the number of the liquid domains. The results show partial melting (~13 %) and superheating of ice occurring at around 20 ns. After 100 ns, the average size of the liquid domains grows from about 2.5 nm to 4.5 nm by the coalescence of approximately six adjacent domains. Subsequently, we capture the recrystallization of the liquid domains, which occurs on microsecond timescales due to the cooling by heat dissipation and results to a decrease of the average liquid domain size.

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Cooperative molecular dynamics of high-density water; dielectric study on glycerol water mixtures under high pressure

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Water is known to exhibit at least two glassy states, high-density-amorphous (HDA) and low-density-amorphous ice, which is thought to be linked to related liquid states. The transformation between glass and liquid states, i.e., the glass transition, of HDA has long been a controversial topic in water physics.[1] Previous studies have been limited due to the difficulty of observing the dynamics of water in a deeply supercooled liquid state, primarily because of unavoidable phase transition. In this study, we employed dielectric spectroscopy, a technique capable of detecting the molecular dynamics of polar molecules such as water, and used glycerol as an additive to stabilize the deeply supercooled state of water to investigate the glass transition of HDA at high pressures of 0.61 and 0.31 GPa and temperatures near the glass transition temperature of the solutions.

Our results reveal two dynamic modes of HDA in the aqueous glycerol solution: one originating from the cooperative motion of water and glycerol involving translational motion with a relatively large relaxation time and another seemingly arising from the local motion of water with a relatively small relaxation time. The concentration-temperature dependence of the relaxation time of the cooperative motion suggests that the glass transition temperature of pure HDA is 150 K at 0.31 GPa and 162 K at 0.61 GPa which consistent with high pressure dilatometry experiments.[2] Moreover, it can be suggested that HDA exhibits a "fragile" glass nature under high pressure, in contrast to its classification as a "strong" glass at 1 atm.[3]

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5-A4-3 16:20-16:40

Neutron Diffraction Study of the Hydrogen-Bond Symmetrization in Ice

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The possibility of hydrogen-bond (H-bond) symmetrization in ice was pointed out more than half a century ago in the paper on the crystal structure of ice VII [1], mentioned as ‘existing well above 22 GPa’. The H-bond symmetrization pressure was first experimentally investigated by infrared and Raman spectroscopy, which is around 60 GPa for H_2O and 70 GPa for D_2O, and this significant isotope effect can be explained by the proton tunnelling through the energy barrier between the two potential minima. The recently reported values for H-bond symmetrization pressure investigated by ^{1}H-NMR and x-ray diffraction rather diverge from 20 to 75 GPa (see [2] and refs. therein). Neutron diffraction could provide definitive information for time- and space-averaged distribution of protons, and the recent neutron diffraction study of D_2O ice VII up to 62 GPa showed that protons are still in non-symmetric states [3]. Here we present our recent results of neutron diffraction for ice VII (or X) taken at the PLANET beamline in MLF/J-PARC using nano-polycrystalline diamond anvil cells [4] and discuss the H-bond symmetrization pressure from the observed proton distribution.

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5-B1-1 9:00-9:30

Exploring the stability and new structures of gas filled ices up to Mbar pressures

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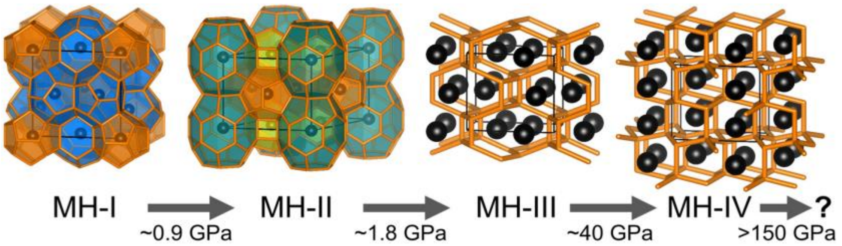

Gas hydrates are overspread on Earth at depth and in the extra-terrestrial space, both interstellar and on outer planets and moons [1-3]. Under the p-T conditions experienced in these medium-size icy bodies, clathrate hydrates adopt filled ice structures whose stability range and properties are still largely unexplored [4-8]. Methane and hydrogen hydrates are also expected to be present under very high pressures (up to 200 GPa) in giant icy planets interior such as in Uranus or Neptune and largely determine their chemistry and conductivity properties. In this talk I will review our recent experimental results - obtained combining neutron and x-ray diffraction, and Raman spectroscopy under high pressure and ab-initio simulations- on gas (H_2, CH_4) [8,9] filled ices under the extreme conditions experienced in the large ice bodies of our solar system.

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Ammonia and clathrate hydrates: phase behavior and structural implications, including incorporation

Mathieu Choukroun[1], Elodie Gloesener[1], Tuan H. Vu[1], Helen E. Maynard-Casely[2], Ashley G. Davies[1], Arnaud Desmedt[3], Christophe Sotin[4]

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Titan, Saturn's largest moon, hosts a 1.5 bar atmosphere where photochemistry constantly dissociates its predominant constituents, methane and nitrogen, which subsequently recombine to form a plethora of organic molecules. The current methane atmospheric amounts would disappear within a few 10s to 100 Myr, thus replenishment mechanisms are necessary to sustain this photochemical cycle over geologic timescales. Methane clathrates are proposed as a likely reservoir of Titan's methane. However, thermal anomalies and/or chemical inhibitors (such as ammonia) would be necessary to release methane from clathrates.

Over the past decade, a growing body of work has suggested that ammonia could be incorporated inside clathrate hydrates, albeit under specific conditions (e.g., 1), in addition to its inhibitory effect on clathrate stability. The exact effect of ammonia on clathrate hydrates remains an area of active research (e.g., 2-6). We will review these recent works in order to clarify the effect of ammonia on the phase behavior of clathrate hydrates, the contexts where incorporation would be expected to occur, and implications for the release of methane from clathrates into Titan's atmosphere.

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5-B1-3 9:50-10:10

Methane – Ethane Substitution in Clathrate Hydrates Studied by Raman Spectroscopy: Implications for the Carbon Cycle on Titan

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Saturn's largest moon Titan is a complex world presenting unique characteristics such as a substantial atmosphere, ongoing organic chemistry and a frigid surface carved by hydrocarbon flows. Clathrate hydrates have long been inferred to constitute a major crustal component of its icy shell, and may contribute significantly to the atmospheric methane's replenishment by releasing their entrapped gas via their dissociation [1-2] or substitution by ethane [3].

In order to better assess the contribution of clathrates to methane outgassing and exchange processes on Titan, it is essential to understand the mechanism of ice-to-clathrate formation and substitution kinetics, which are currently poorly constrained. In this study, we carry out Raman spectroscopic investigations of the CH_4-C_2H_6 replacement kinetics in clathrate hydrates at pressure and temperature conditions relevant to Titan. Our results show the successful formation of ethane clathrate hydrates from the reaction of liquid ethane with methane clathrates and ice. This supports the hypotheses that liquid ethane can be trapped in Titan's subsurface and that methane could be released as ethane replaces it in clathrate hydrates.

This work has been conducted at the Jet Propulsion Laboratory, California Institute of Technology, under contract to NASA. Government sponsorship acknowledged.

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5-B2-1 10:30-10:50

Complete Low Pressure (80 bar) Cycling of Hydrogen in Pure Hydrogen Hydrate: Toward Gas Storage

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Clathrate hydrates (also recently referred to as zeolitic ice) are well known to contain methane, carbon dioxide and hydrogen and are of current research interest regarding climate mitigation. Pure hydrogen clathrate hydrate (H2 and H2O), formed by trapping hydrogen in water-cages, has great potential for high volume hydrogen storage (5 wt % hydrogen). However, the biggest drawback is the inability to cycle hydrogen because the clathrate structure collapses when the hydrogen is removed, thus requiring high hydrogen pressure, 1.8 kbar, be applied to form new clathrate material. Here, we show that hydrogen can be completely removed from the hydrate while maintaining empty zeolitic ice XVI. This pre-formed clathrate structure lowers the energy barrier for hydrogen hydrate synthesis, only requiring hydrogen pressure 80 bar. The new hydrate sample has singly occupied small cages and triply occupied large cages, giving a hydrogen to water molecular ratio as high as 40 H2 : 136 H2. This demonstrates low pressure hydrogen cycling.

Formation of mixed hydrate to separate CO_2 from R134a + CO_2 gas mixture for LNG gasification unit

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Regasification of LNG in FSRU (Floating Storage Regasification Unit) requires highly efficient refrigerant due to space limitation. 30 mol% glycol solution has been widely used for the regasification unit, however it requires more than 500 ton/hr for the regasification of 100 ton/hr of LNG, demanding large size heat exchangers. From the process simulation, R134a+CO2 gas mixture only requires 270 ton/hr for LNG gasification, thus compact design becomes feasible. Both R143a and CO2 are one of the strong green-house gases, separation of both R143a and CO2 must be considered during the maintenance of the regasification unit. Cryogenic distillation is the popular option to separate CO2 from the gas mixture, recent findings strongly suggest that gas hydrates formation might be beneficial to separate CO2 from R134a+CO2 gas mixture. As R134a is the hydrate promoter shifting the hydrate formation condition, most hydrate cages would be filled with R134a molecules. In this work, gas hydrate was formed from R134a+CO2 gas mixture and the composition of gas phase was analysed to develop the concept of stepwise hydrae-based separation process. To obtain ~ 90 mol% CO2, it requires at least three stages of hydrate formation and dissociation. Then the recovery ratio of the hydrate-based separation process was compared to those of cryogenic distillation processes varying pressure from 1.3 to 13 bar. The obtained results suggested that the hydrate-based process showed better separation efficiency.

Effect of injecting pressure on CO_2 exchange behaviors into C_3H_8 hydrate

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Natural gas hydrates (NGHs) are our future clean energy resources with a greater energy density. NGHs usually have sI hydrate structure due to CH_4 is a primary component of natural gas and it is sI hydrate former. When larger hydrocarbons enter the hydrate phase more than common composition of natural gas, NGHs also form sII or sH hydrates depending on the type of the guest. C_3H_8 is one of the major components of natural gas that induce the sII hydrate structure with empty small cages. In the previous works, the guest replacement in sII hydrates with CO_2 or various compositions of CO_2 + N_2 feed gases were studied each mechanism that partial-structural transition or iso-structural transition is occurred depending on the feed gas compositions. To elucidate the influence of the replacement of C_3H_8 and CO_2 on the extent of structural transition, the enclathrating behaviors of the guests were examined by qualitative analysis of each phase and structural analysis under different CO_2 injecting pressures. The guest compositions in the vapor and hydrate phases were measured using a gas chromatograph. PXRD analyses coupled with Rietveld refinement were used on each hydrate sample to calculate weight fractions of each phase and cage occupancy of guest molecules after the replacement under different CO_2 injecting conditions. The results showed that the compositions in the hydrate remained almost constant before a specific injecting pressure, which showed non-transition of the sII hydrates to sI hydrates. If the pressure above a critical point, the CO_2 composition in the hydrate phase increased drastically and the structural transition to the sI hydrate occurred. The guest compositions in the hydrate phase via GC corresponded well with those obtained by PXRD analyses at each injecting pressure. The findings from this study would be helpful for understanding the role of C_3H_8 in determining the stable structure and the efficiency after the replacement.

5-B2-4 11:30-11:50

Crustal fingering facilitates free-gas methane migration through the hydrate stability zone.

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Widespread seafloor methane venting has been reported in many regions of the world oceans in the past decade. Identifying and quantifying where and how much methane is being released into the ocean remains a major challenge, and a critical gap in assessing the global carbon budget and predicting future climate. Methane hydrate forms from methane-water mixture under elevated pressure and low temperature conditions typical of the deep marine settings (>600 m depth), often referred to as the hydrate stability zone (HSZ). Wide-ranging field evidence indicates that methane seepage often coexists with hydrate-bearing sediments within the HSZ, suggesting that hydrate formation may play an important role during the methane gas migration process. At a depth that is too shallow for hydrate formation, existing theories suggest gas migration occurs via capillary invasion and/or initiation and propagation of fractures. Within the HSZ, however, a theoretical mechanism that addresses the way in which hydrate formation participates in the gas percolation process is missing.

In this work, we study, experimentally and computationally, the fluid mechanics of gas percolation under hydrate-forming conditions. We uncover a new phenomenon --- crustal fingering --- and demonstrate how it may control methane gas migration in ocean sediments within the HSZ. We extrapolate the underlying physics of this phenomenon to understand its implications at the scale of multiple methane seeps. Our field-scale simulations suggest that the crustal fingering mechanism could help interpret intermittent temporal dynamics of deep methane seeps, trace the origin of hydrate fabrics in the subsurface environment, and advance our understanding of hydrate-seep interactions in the past and future climate.

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5-B3-1 13:30-13:50

On the thermodynamic stability of CH_4-CO_2 binary hydrates under multiple coexistence of water, hydrate, and guest fluids.

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We have developed a method to evaluate the thermodynamic stability of clathrate hydrates relative to host water and/or guest species. This enables to investigate complete phase behaviors of hydrates in the whole space of the thermodynamic variables, not only temperature and pressure but also composition, with only the intermolecular interactions as input parameters. A complete phase diagram of hydrate is settled with this method, specifically the region enclosed by the hydrate/water and hydrate/guest phase boundaries where a hydrate is the only stable phase. The method is applied to various hydrate, which results in an excellent agreement in dissociation pressure with the experimental observations [1,2].

Here, we apply the above theory to CH_4-CO_2 binary hydrate. The free energies of cage occupations allow us to connect the chemical potentials of the individual components to the compositions of guest, leading to the phase behaviors as well as the cage occupancies in the whole space of thermodynamic variables. We have used only several empirical parameters, the critical temperatures and pressures of CH_4 and CO_2, and the factor to adjust unlike interaction between CH_4 and CO_2 molecules. The chemical potentials of water and guest species are all calculated once the intermolecular interactions are given.

It is found that a difference in the affinities of each guest species to the larger and smaller cage of the binary hydrate affects significantly occupation of each cage type which results in a deviation of the composition of guest in the hydrate from that in the fluid at the two-phase equilibrium conditions. Also, the two-phase coexistence of the fluid mixture in equilibrium with the hydrate alters the hydrate/fluid boundary and the occupancies of each guest in two sorts of cages at low pressures.

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5-B3-2 13:50-14:10

Metastability of carbon monoxide and nitrogen gas hydrates from first-principles calculations

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At a fundamental level, the nano-structuration of gas hydrates confers on these materials specific physico-chemical properties. The understanding of their molecular interactions plays a key role in the future developments – requiring to combine advanced experimental and modeling approaches. Metastability is one of those fascinating properties. Gas hydrates (e.g. carbon monoxide or nitrogen) may form into one type (sI structure) and transform to another type (sII structure) over duration ranging from hours to months, as revealed by means of time-dependent and in situ neutron diffraction experiments [1,2].

In this work, quantum mechanics modeling using density functional theory (DFT) have been performed to unravel metastability properties of CO and N_2 clathrate hydrates. In particular, it is shown that metastability is associated with the ability of gas hydrates to catch two guest molecules in the larger cages of sII structure. The presentation will review these recent results [3,4] focusing on DFT-derived structural and energetic properties along with pressure effect.

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Rotations of Methane Molecules in Amorphous and Crystalline Hydrates

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Methane hydrate has been studied extensively not only as a future energy resource but also from the interest in quantum and classical rotations of methane molecules. In this study, amorphous methane hydrate (a-MH) [1] was formed by vapor deposition at 5 K using a custom-made cryostat [2] and its quasi-elastic neutron scattering (QENS) and inelastic neutron scattering (INS) data were collected at 5 to 80 K using AGNES spectrometer at JRR-3, Tokai, Japan. The QENS and INS data of the crystalline methane hydrate (c-MH) were also measured for the sample annealed at 150 K.

Figure 1 shows clear QENS data due to the methane rotation in a wide temperature range from 5 to 80 K. The data were well fitted to a Lorentz function and the relaxation time τ was calculated from the peak width. Similar QENS data were observed also in c-MH. The Arrhenius plot (Fig. 2) shows that the a-MH has longer τ than c-MH. This is probably because of the narrow and disordered cage spaces in a-MH. It is of interest that there is a clear bending of the τ line around 20 K for both samples and the slope in the low-temperature side is very small. We guess that there is a crossover between the classical (high-T) and quantum (low-T) rotations around 20 K. Additional neutron diffraction and calorimetric works are now going on.

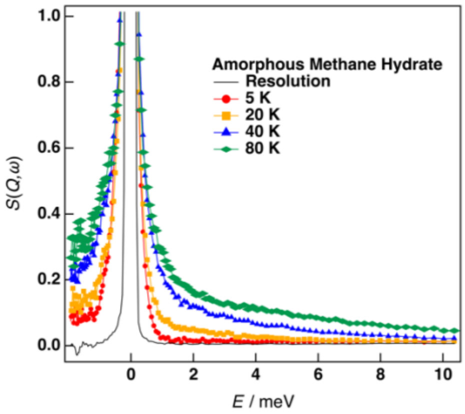

Fig 1. QENS spectra of a-MH.

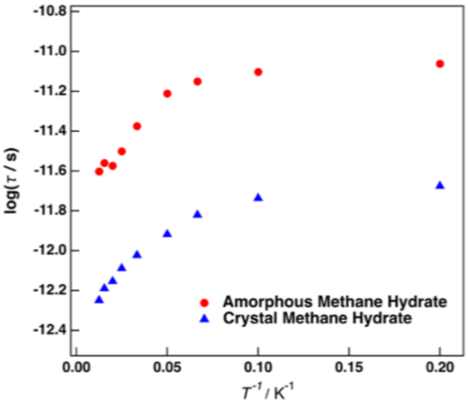

Fig. 2. Arrhenius plots of a-MH and c-MH.

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5-B3-4 14:30-14:50

Proton conduction mechanism in TBAB semiclathrate hydrate obtained by NMR and QENS measurements

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Semiclathrate hydrate (SCH) is a crystalline inclusion compound, in which a quaternary onium cation is incorporated into hydrate cages made from host water molecules and anions. The anions join in the hydrogen-bonded networks with the water cages. Tetra-*n*-butylammonium bromide (TBAB) is a typical guest for SCH.

We investigated the proton conductivity in single-crystalline TBAB SCH by electrochemical impedance spectroscopy (EIS).[1] The conductivity in TBAB SCH was much higher than that in hexagonal ice. This result suggests that TBAB SCH has a higher mobility of protons, causing water dynamics to differ from hexagonal ice.

In order to reveal the conduction mechanism in TBAB SCH clearly, nuclear magnetic resonance (NMR) and quasi-elastic nuclear scattering (QENS) measurements were performed. As the result, we observed the reorientation motion of water molecules through the relaxation times of the μs-order (by NMR) and ps-order (by QENS). The reorientation motion with ps-order (by QENS) would mean that the reorientation of water around anions. The relaxation time with μs-order (by NMR) agrees with the electrical relaxation time of proton conduction (by EIS), *i.e.*, the water reorientation with μs-order is the rate-limiting step for the proton conduction in TBAB SCH.

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5-B3-5 14:50-15:10

Homogeneous and Heterogeneous Nucleation of Clathrate Hydrates under Non-equilibrium Conditions with Time and Temperature Resolved Synchrotron X-ray Diffraction

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Clathrate hydrates are nonstoichiometric framework compounds composed of water molecules with guests encapsulated in the cages formed through a network of hydrogen bonds. Hydrates formed from small hydrocarbon molecules are abundant on Earth. Gas hydrates are believed to exist in the Solar system or even exoplanets. The prevalence of clathrate hydrate in the universe raises questions on how and when they are formed under non-equilibrium thermodynamic conditions. To study this problem, we have constructed a cryogenic vapour deposition system to mimic conditions of the interstellar medium and allow simultaneous measurements of the diffraction pattern and Raman spectra at a synchrotron. We have studied several heterogenous and homogenous guest-water systems. A general trend in hydrate formation associated with the sequence of structural transformations of amorphous ice was observed. Using total diffraction, we captured the temporal structural rearrangement of a xenon/ water mixture from total diffraction analysis. We will also report results on other guest-water systems.

5-B4-1 15:30-16:00

Insights from Structure and Chemical Reactivity of Water Adsorbed on Particle Surfaces

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The gas-particle surface is of essential importance as it directly determines many atmospheric processes, *e.g.*, trace gases uptake, redox reactions, ozone depletion and heterogeneous ice nucleation. Surfaces may spontaneously undergo unexpected chemical reactions that are thermodynamically unfavored when water is present. For example, a surface-catalyzed redox mechanism was discovered when a salt surface was observed in its initial solvation stages, as water was adsorbing [1]. Like the previously discovered “on-water” catalysis (aqueous phase surface water) [2], the new mechanism can be described as “water-on” surface catalysis (surface water adsorbed from the gas phase).

Upon water adsorption, aerosol particles surfaces can provide chemically active environments that facilitate thermodynamically unfavored reactions, similar to the catalytic environment on the surfaces of ice particles [3]. These processes are challenging to characterize, and therefore advanced surface-sensitive experimental techniques like synchrotron-based ambient pressure X-ray photoelectron spectroscopy (APXPS) are utilized to investigate the interfacial environments. We present a series of APXPS studies to illustrate how water structures on salt surfaces, and how this influences the chemically reactive environments on these surfaces.

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5-B4-2 16:00-16:20

Experimental characterization of the NO_2/N_2O_4 hydrolysis reaction intermediates on ice

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The hydrolysis of NO_2 at the air/ice interface plays an important role in regulating the oxidative capacity of the atmosphere. Indeed, the reaction yields nitric acid and nitrous acid, compounds which acidify precipitations, but which also creates photochemical sources of NO_x and OH radicals. In the gas phase, NO_2 is at equilibrium with its dimers, N_2O_4, which can exist in the form of constitutional isomers and stereoisomers, but whose abundance and reactivity towards hydrolysis continue to be debated. These uncertainties regarding the reaction mechanism, along with the lack of adequate and relevant experimental data to describe these processes, whether within the ice or at its surface, hamper heterogeneous NO_2 hydrolysis to be accurately accounted for in atmospheric chemistry models.

Using Electric Field Standing Waves (EFSW) to enhance the sensitivity and selectivity of Reflection-Absorption IR Spectroscopy (RAIRS), along with molecular beam deposition methods, it is shown that the chemical speciation in NO_2 vapours can be greatly modulated by heating or cooling the nozzle yielding various ratios of the NO_2 monomer and of its dimer, N_2O_4. More importantly, it also allows control over the distribution of *cis*-$ONONO_2$ and *trans*-$ONONO_2$ metastable isomers of N_2O_4 in NO_2 vapours. As the relative abundance of metastable *trans*-$ONONO_2$ is observed to increase upon heating of the molecular beam nozzle, its reactivity towards heterogeneous hydrolysis on ice can be assessed directly. Recent progress in the molecular-level understanding of this reaction will be presented, which could improve the accuracy for atmospheric models.

5-B4-3 16:20-16:40

Isotopic Constraints on Snow Nitrate Photolysis in Inland East Antarctica: Knowns and Unknowns

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Nitrate is one of the most abundant chemical species in Antarctic snow and ice and is widely measured in previous studies [1]. The interpretation of nitrate in ice core, however, remains challenging due to photolytic loss of nitrate after deposition, especially in low snow accumulation sites (e.g., inland East Antarctica). Theoretical as well as lab and field studies all agree that ^{15}N will be strongly enriched in nitrate that remains in snow after major photolytic loss [2,3], while δ^{18}O and Δ^{17}O decrease with nitrate photolytic loss generally attributed to secondary chemistry at the ice crystal surface where the photoproducts can exchange oxygen atoms with water [4], but the mechanism has yet to be quantitatively assessed despite its importance for interpreting ice core records. Here we contribute new insight using a model simulating isotopic fractionation associated with NO_3^- burial, photolytic loss, and re-oxidation in snow. We find that photolysis-driven aqueous-phase formation of secondary nitrate is on the order of ~25-30%, and isotopic effects of nitrate photolysis and aqueous-phase re-oxidation chemistry are important sources of uncertainties in modelling δ^{18}O.

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3) Shi G., Buffen A.M., Hastings M.G., Li C., Ma H., Li Y., Sun B., An C. and Jiang S. *Atmos. Chem. Phys.* **15**, 9435–9453 (2015).
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6-A1-1 9:00-9:20

Polyamorphism in vitrified water droplets: nucleation of a liquid in a liquid

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Water is one of the few anomalous substances and one of the few substances that exhibits polyamorphism. Three distinct amorphous ices, low- (LDA), high- (HDA) and very high-density amorphous ice (VHDA) are distinguished [1]. The liquid–liquid critical point model explains the anomalies based on two liquids, where HDA and LDA are considered glassy proxies [2]. Yet, experimental evidence supporting the link between amorphous ices and supercooled liquids is contested. According to some researchers, the procedure to make LDA/HDA (that starts from crystalline ice) [3] rather yields a nanocrystalline solid unrelated to glasses [4]. In our work we instead start from liquid water droplets, which are cooled at 10^7 K/s so that they turn into a solid composed of glassy droplets, called hyperquenched glassy water (HGW) [5]. We demonstrate that HGW experiences a sharp glass-glass transition to the densified glass (d-HGW) at < 120 K [6]. We furthermore identify two distinct glass transition temperatures, i.e., these two types of glassy materials develop into two distinct, viscous liquids upon heating. This provides strong evidence that amorphous ices are thermodynamically connected to liquids and not to nanocrystals. In terms of molecular structure HGW and d-HGW are very closely related to LDA and HDA. Use of appropriate annealing protocols allows us to study the viscous liquids at 1 bar up to 141 K [7]. This corresponds to the highest stability achieved so far for bulk water and has allowed us to observe the novel phenomenon of nucleation of the low-density liquid in the high-density liquid at 137 K as a spike in heat capacity.

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6-A1-2 9:20-9:40

Revealing the Dynamics of High-Density Amorphous Ice Using X-Ray Photon Correlation Spectroscopy

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Water is the key component for the existence of life on Earth and plays a central role in a wide range of scientific disciplines, such as biology, chemistry, atmospheric chemistry, and geophysics. The existence of two liquid phases (high- and low-density liquid (HDL, LDL)) has been proposed to explain the origin of the anomalous properties of water. The two liquid states are thought to be the counterparts of high- and low-density amorphous ices (HDA and LDA), respectively. However, the dynamics and structural nature of amorphous ice are still controversial.

X-ray photon correlation spectroscopy (XPCS) has been used as a powerful technique to probe the dynamical properties of free-standing amorphous ices [1]. To reveal the mechanism of water´s phase transitions and the interconnection between amorphous ices and liquid water, we combine wide-angle X-ray scattering (WAXS), ultra-small-angle X-ray scattering (USAXS) and XPCS to probe both the structural and dynamical properties of amorphous ices during the HDA-LDA transition. In our thin samples, we unexpectedly observe a heterodyne signal, which we assume to be related to island of static LDA or crystalline ice floating in a matrix of HDL. I will also give an outlook to our recent in-situ high-pressure experiments.

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6-A1-3 9:40-10:00

Topological analysis on amorphous ices using persistent homology

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Water has at least two distinct amorphous solid states: low-density amorphous ice (LDA) and high-density amorphous ice (HDA) [1]. These are considered to be different thermodynamic amorphous phases due to the first-order phase transition-like behavior to pressure between them. In addition, two amorphous states can be made from HDA: eHDA, the structural relaxation state of HDA at low pressure [2], and VHDA, the state which HDA is annealed at high pressure [3]. Although various amorphous phases of ice have been proposed, it is still unclear whether these amorphous states are thermodynamically different phases and whether they can be clearly distinguished structurally.

In this study, topological analysis using persistent homology is conducted on the atomic configurations of various amorphous ices reproduced from computer simulations using TIP4P/2005 potential [4] to characterize these amorphous structures. Persistent homology, a new topological analysis method, enables a hierarchical understanding of ordered structures at various scales and has proven to be a powerful analytical tool for amorphous structures, where medium range ordered structures are considered essential [5]. Using this method, we revealed the topological differences between eHDA and VHDA, which have not been clarified up to date.

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6-A1-4 10:00-10:20

Structure and Phonon Excitations of Vapor-deposited Amorphous Ice and Their Annealing Effects Studied by X-ray/Neutron Scattering Techniques

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Kazutaka Ikeda[2], Maiko Kofu[3]

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Amorphous Ices are realized by various methods, e.g., vapor deposition, micro-droplet quenching, compression of crystalline ice, etc. They are in non-equilibrium state and so structurally relaxed to more stable amorphous or crystalline states if they are sufficiently thermally activated. In the present study, we have formed vapor-deposited amorphous ices using custom-made cryostats [1,2] and investigated their annealing temperature dependences of the structure and phonon vibration states using an X-ray diffractometer (in-house), neutron diffractometer (NOVA, MLF, J-PARC), and inelastic neutron scattering instrument (AMATERAS, MLF, J-PARC).

From the X-ray and neutron diffraction data, we have calculated the temperature dependence of pair distribution functions and found that the hydrogen-bonded network is more developed by annealing at higher temperatures. It is of interest that the structure relaxation occurred even at 80 K, which is much lower than the glass transition temperature (ca. 130 K). Figure 1 shows the $S(Q,E)$ map of the amorphous D_2O ice which was annealed at 120 K. There is a clear dispersion-like phonon below 10 meV. The dispersion curves seem to originate at the Q positions of the peak of $S(Q)$ as in crystalline D_2O ice. This is quite unusual since there is no unit cell in the amorphous ice. We will discuss the relation between the network structure and phonon excitations.

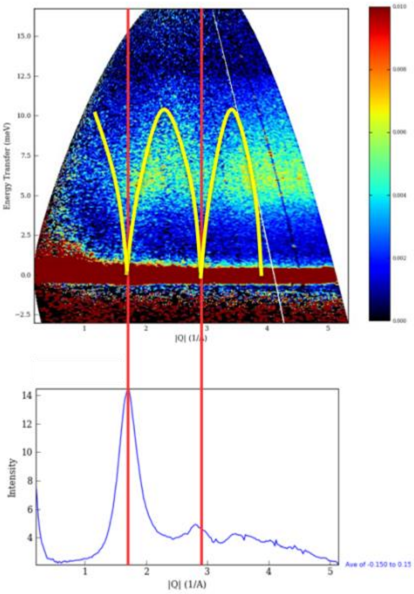

Fig. 1 $S(Q,E)$ map of a-D_2O ice

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In-situ observation of pressure-induced amorphization of methane/ethane hydrates by vibrational spectroscopy

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Pressure-induced amorphization (PIA) of ice and clathrate hydrates undergoes at the low temperatures far below their melting or decomposition points. We have investigated the PIA of the type I clathrate hydrates containing methane and ethane as guest molecules by using Raman and infrared (IR) spectroscopies. On isothermal compressions at 100 K, methane hydrate (MH) undergone PIA at 2.5–3.5 GPa, while ethane hydrate (EH) undergone at 4.0–5.0 GPa. The type I clathrate structure consists of two types of cages: small (5^{12}) and large ($5^{12}6^{2}$) cages. Comparison of the spectra of both amorphized iso-structural hydrates allows us to gain an insight into the effect of the size of the guest molecule on the collapse process and their amorphous forms.

The Raman results revealed that the collapsed small and large cages in amorphous forms of MH and EH are not distinguished. The collapsed cages including methane and ethane molecules are similar with small and large cages, respectively. Their water-networks are folded or expanded in the process of the PIA so that the cavity sizes of collapsed cages are compatible with those of the guest molecules. For the IR spectra of crystalline MH, IR peaks assignable to the ro-vibrational transition of methane in the large cages were observed in the C-H stretching wavenumber regions below 40 K [1,2]. The ro-vibrational IR band was disappeared after amorphization. This suggests that the rotational motion of methane molecule in the large cage is frozen by collapsing, as had been reported by previous dielectric spectroscopic and simulation studies. This study will contribute to better knowledge for changing of the local structure around guest molecules during the PIAs and the dynamics of guest molecules.

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A systematic study of the influence of the ice formation temperature on spectroscopic properties of methanol interstellar ice analogues

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As a simple organic compound, CH3OH can be a component in many reactions in the Interstellar Medium (ISM) leading to compounds such as methane, formaldehyde, ethylene glycol, or dimethyl ether [1]. However, not only is methanol's reactivity worth further research, but also its structure. With the first phase transition at the temperature of 103 K [2], methanol ice can occur both in the amorphous, or crystalline form [3].

As there is still a lack of detailed, systematic studies on methanol ice's properties, this research is focused on its crystalline structure as a function of temperature. In this study, CH_3OH ice layers were grown in the Portable Astrochemistry Chamber (PAC) with the ability to control deposition pressure and temperature. Several experiments were performed to investigate the behavior of phase transition under different conditions and to analyze the influence of the ice formation process on vibrational spectra.

Two vibrational modes were chosen for analysis of the methanol ice structure: OH stretch and CO stretch. It was observed that differences in mid-infrared (mid-IR) spectra were visible depending on ice formation temperature, which shows applicational potential for studies of thermal history and more detailed astronomy observations. A Principal Component Analysis (PCA) method had been chosen to create a chemometric model enabling recognition of the temperature of ice formation based on the mid-IR spectrum of methanol ice.

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3) E. S. Wirström, W. D. Geppert, Å. Hjalmarson, C. M. Persson, J. H. Black, P. Bergman, T. J. Millar, M. Hamberg, E. Vigren, *A&A*, **533**, A24 (2011).

6-A2-3 11:20-11:40

Accurate Crystal Structures of Ices from X-Ray and Electron Diffraction with Hirshfeld Atom Refinement

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We applied Hirshfeld Atom Refinement (HAR) of single crystal high pressure (sc HP) X-ray synchrotron and laboratory X-ray and electron diffraction data. This method utilizes aspherical atomic scattering factors (X-rays), and aspherical atomic electrostatic potentials (ED), based on so called stockholder (Hirshfeld) partition and is especially effective in the case of refinement of crystals of H-rich compounds.

We present accurate crystal structures of H_2O, D_2O and mixed (50%H_2O/50%D_2O) ice VI and ice VII obtained by HAR against sc HP synchrotron and laboratory X-ray diffraction data as well as results of refinement of hexagonal ice obtained by HAR against electron diffraction data (Fig. 1). It was possible to obtain O-H bond lengths and anisotropic ADPs for disordered hydrogen atoms which are in good agreement with the corresponding results of single crystal neutron diffraction data.[1] Our results show that HAR against X-ray diffraction and electron diffraction data is a tool which can compete with neutron diffraction in detailed studies of polymorphic forms of ice and crystals of other hydrogen rich compounds. Cheaper and more accessible X-ray measurements combined with HAR can facilitate the verification of the existing ice polymorphs and the quest for the new ones.[1]

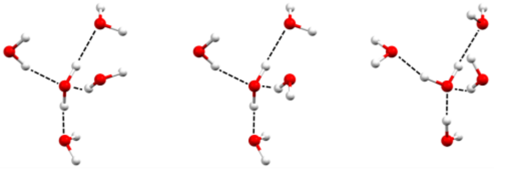

Fig 1. Examples of water clusters (259 in total) considered for ice VI.

1) M. L. Chodkiewicz, R. Gajda, B. Lavina, S. Tkachev, V. B. Prakapenka, P. Dera, K. Woźniak, *IUCRJ*, **9**, 573-579 (2022).

Financial support of this work by the National Science Centre, Poland, through OPUS 21 grant number DEC-2021/41/B/ST4/03010 is gratefully acknowledged.

6-B1-1 9:00-9:20

The inherent chemical reactions occurring within ice and their consequential implications and potential applications

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Ice is an essential and omnipresent reaction medium in the environment. According to the *Arrhenius Equation* ($k=A\cdot e-EA/RT$), chemical reactions theoretically proceed slowly as temperature decreases, but recent research has shown that several chemical reactions are actually accelerated by freezing compared to those in water. This phenomenon is attributed to *the Freeze Concentration Effect*, whereby organic and inorganic compounds are separated from ice crystals and highly concentrated in unfrozen parts or ice grain boundaries.

In this talk, we aim to introduce accelerated reactions in the frozen state and their impact on climate change. First, we discuss the enhanced dissolution of metal oxide and clay minerals in ice, leading to novel processes for the formation of new minerals. Next, we explore the accelerated chemical transformation of iodine species in the frozen state. Additionally, we examine the chemical transformation or removal of environmental pollutants in ice.

The presentation will delve into the research background, experimental conditions, mechanistic explanation, and effects on climate change associated with these processes. By examining the unique chemical reactions that occur in ice, we can gain a better understanding of the environmental impacts and how they contribute to climate change. This presentation promises to deliver insightful knowledge regarding the multifaceted impact of ice chemistry on the environment, its consequential effects on our planet, and its potential applications to benefit humankind.

Quantitative study of freezing concentration in polycrystalline ice crystals upon ice recrystallization

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Contrary to the conventional concept that chemical reactions slow down as the temperature of the system decreases according to the Nernst equation, it has been reported over the past decade that certain chemical reaction rates increase in ice phase. The key to this unique reaction is the "freeze-concentration effect". In polycrystalline ice, chemicals dissolved in water are concentrated at the ice grain boundaries, known as the quasi-liquid layer (QLL). Ice in the natural environment is exposed to temperature changing cycles ranging from days to months, and these temperature changes accelerate ice recrystallization, resulting in chemical concentration changes and migration at the QLL.

In this study, we aimed to quantitatively analyze the distribution and concentration changes of chemicals in QLLs during ice recrystallization. Using cryo-Raman spectroscopy, we found that asymmetric hydrogen bonding at the ice interface increases as the concentration of NaCl in the QLLs increases during the ice recrystallization process. In addition, using confocal microscopy, the fluorescent molecules gathered into the ice grain boundaries, migrated and concentrated during the ice recrystallization process. As the temperature cycle was repeated, the growth of ice crystals through recrystallization increased, as the concentration of the chemicals into the QLL increase. These results could provide a deeper understanding in chemical reaction mechanism in polycrystalline ice undergoing recrystallization in the natural environment.

6-B1-3 9:40-10:00

TEM study on the evolution of micro-cavities in ice by electron radiolysis

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Upon electron irradiation, cavities are formed in ice due to immediate clustering of myriad vacancies generated by diffusion of hydrogen and oxygen atoms from their lattice sites, which are a direct result of radiolysis of water by high-energy incident electrons [1]. The cavity is probably filled with ionized gas generated by the radiolysis [2]. With a liquid cell transmission electron microscopy (LC-TEM), we studied a time-evolution of micro-cavities in ice at the moments of their formation, through the coalescence, and up to their rupturing.

Figure 1 shows time-evolutions of micro-cavities in ices around -15 °C obtained by a 200 keV TEM (JEM-2100F). The ice always disappears gradually from a sight by electron radiolysis loss of the ice and sublimation of the ice caused by slight temperature elevation. We found that size and shape of the micro-cavities and evolution path of the micro-cavities were changed depend on the thickness of their mother ices that estimated from 50 to 900 nm. The ice thicknesses were estimated by an equation, $d = -ln(I(d)/I_0)\lambda E$ under two assumptions: The primary intensity (I_0) correspond to the average electron intensity of selected five brightest points in each subfigure of Fig. 1; The primary electron is decayed just by inelastic scattering of electron though ice of the thickness of d. Values of the inelastic mean free path (λE) are adopted from a reference [3].

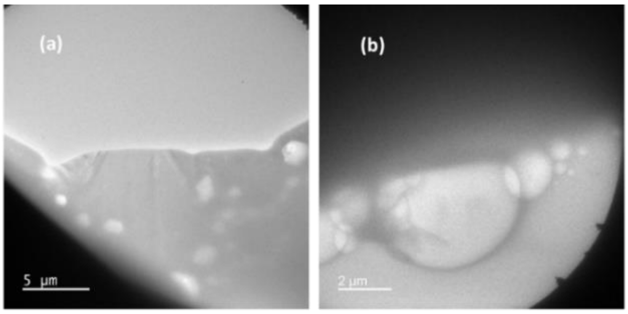

Figure 1. Bright field TEM image of a selected frame of each video of micro-cavities evolution in ice encapsulated between electron-transparent SiN windows. The relatively dark fields correspond to ice with variable thickness from 50 to 900 nm and the relatively bright fields are filled with ionized gas generated by the radiolysis.

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6-B1-4 10:00-10:20

Identification of a permanent reservoir of bromine in Arctic snow in the form of bromate (BrO_3^-).

Stefano Frassati[a], Elena Barbar [a,b], Giulio Cozzi[a,b], Clara Turetta[a,b], Federico Scoto[c], Alfonso Saiz-Lopez[d], Kitae Kim[e], Ward van Pelt[f], Carlo Barbante[a,b], Andrea Spolaor[a,b]

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Bromine (Br) and iodine (I) are chemical species that play central roles in polar atmospheric chemistry, ozone depletion, and cloud condensation nuclei formation and the natural sources to the atmosphere is the ocean[1]. In particular, bromine undergoes a series of autocatalytic reactions that lead to sunlight-induced ozone depletion, these reactions are known as "bromine explosion"[2]. This catalytic cycle occurs at the air-snow interface, but currently, photochemical reactions are only included in the gas phase and possible photo-oxidation of bromine in snow is not addressed.

In this study, an analytical method for the speciation of Br and I was developed by ion chromatography system (IC) coupled with inductively coupled plasma sector field mass spectrometer (ICP-SFMS). Thanks to this instrumental set-up we were able to achieve detection limit (LOD) of 0.3 pg g^{-1} for I^-, 1.13 pg g^{-1} for IO_3^-, 3.6 pg g^{-1} for Br^-, and 2.1 pg g^{-1} for BrO_3^-, respectively. This analytical method has been used to analyze snow samples from Holtedahlfonna glacier (HDF, Svalbard Islands) collected in interval of 10 cm. For the first time, through fine-tuning of IC/ICP-SFMS technique, it was possible to detect bromate (BrO_3^-) in Artic snow at pg g^{-1} level. The most interesting result is that the concentration of BrO_3^- remains almost constant in the deepest samples corresponding to the polar night period, but there is a significant increase in the layers exposed to sunlight. This mean that oxidation processes of bromine could occur into the snowpack producing, although in low percentage, a reservoir of inactive bromate species.

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2. Pratt, K. A. *et al.Nat. Geosci.* **6**, 351-356 (2013).

6-B2-1 10:40-11:00

Methanol production through the impingement of low-energy CH_3^+ ions onto an ice surface at low temperature

Y. Nakai[1], W. M. C. Sameera[2,3], K. Furuya[4], H. Hidaka[2], A. Ishibashi[2], and N. Watanabe[2]

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Many theoretical and experimental studies have been performed to reveal production pathways of various chemical species in molecular cloud. Ion-molecule reactions in gas phase are thought to be indispensable. Reactions of hydrogen atoms adsorbed on icy grain have also been shown to be essential for productions of abundant molecules such as hydrogen, water, and methanol [1]. Besides these reactions, recent theoretical studies have suggested molecular formation via reactions of low-energy ions with ice surface as a new reaction pathway [2]. In contrast, little experiments have been performed because of experimental difficulties. We have developed an experimental apparatus using pick-up method by low-energy Cs^+ ions for detection of reaction products on ice surface [3].

The CH_3^+ ions in the energy range of several electron volts impinged on the surface of amorphous solid water. After CH_3^+ irradiation, the products of methanol molecules were observed as the theoretically suggested. In addition, we investigated ice-temperature dependence of methanol production via ion-ice surface reactions. Little temperature dependence of methanol yields is observed in the temperature range 12–60 K. Ab-initio molecular dynamics simulations with NVT ensemble at 10 K suggested that methanol molecules are produced spontaneously, without regard to the contact points of the CH_3^+ ions. From an astrochemical model simulation [4], we found that the influence of this reaction on the methanol abundance is limited at the edge of molecular cloud.

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2) D. E. Woon, *Acc. Chem. Res.*, **54**, 490-497 (2021).
3) H. Kang, Bull. *Korean Chem. Soc.*, **32**, 389-398 (2011).
4) K. Furuya, et al., *Astron. Astrophys.*, **584**, A124 (2015).

6-B2-2 11:00-11:20

Visible Light Induced Photodesorption of Hydroxyl Radicals from Amorphous Solid Water

Masashi Tsuge[1], Ayane Miyazaki[1], Ni-En Sie[1], W. M. C. Sameera[1], Y. Nakai[2], Tetsuya Hama[3], Hiroshi Hidaka[1], Akira Kouchi[1], Naoki Watanabe[1]

[1]Institute of Low Temperature Science, Hokkaido University, N19-W8, Kita-ku, Sapporo 060-0819, Japan, [2]Radioactive Isotope Physics Laboratory, RIKEN Nishina Center, Wako, Saitama 351-0198, Japan, [3]Komaba Institute for Science, The University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan

In very cold and dense interstellar regions, so-called molecular clouds, more than 150 kinds of molecules have been identified. It has been suggested that the surface reactions on dust grains play very important roles in molecular formation. In the cold regions with temperatures as low as 10 K, the surface of dust grains are typically covered predominantly with amorphous solid water (ASW). Because hydroxyl (OH) radicals are an intermediate of H_2O formation and a photolysis product of H_2O, the OH radical is one of the dominant radical species on icy dust. Thus, a better understanding of the their behavior on ASW is important in revealing molecular formation towards larger species. However, the detection of OH radicals on the surface has intrinsic experimental difficulties due to their high reactivity. In this work, we developed a sensitive, surface-selective, and species-selective method for the detection of OH radicals on ASW [1].

We combined the photostimulated desorption and resonance-enhanced multiphoton ionization techniques for the detection of OH radicals and found that OH radicals can be photodesorbed from ASW by a visible photon at 532 nm, where both isolated OH radical and H_2O molecule are transparent. Quantum chemical calculations addressing an OH radical adsorbed on ASW indicated that the valence A–X transition of OH radical is significantly red-shifted when the OH radical is strongly adsorbed to ASW through three hydrogen bonds. We are currently studying the wavelength dependence of OH radical photodesorption yield in the visible region. Because the yield is determined by the absorption cross-section and quantum yield of desorption, we may be able to obtain the absorption spectrum of OH radicals on ASW with the aid of quantum calculations.

1) A. Miyazaki, N. Watanabe, W. M. C. Sameera, et al., *Phys. Rev. A*, **102**, 052822 (2020).

6-B2-3 11:20-11:40

Gas-Ice Partitioning Coefficients of Carbonyl SOA precursors during Diffusional Ice Crystal Growth

Jackson Seymore[1,2], Miklós Szakáll[2], Alexander Theis[3], and Subir Mitra[3]

[1]Max Planck Graduate Center, Institute for Chemistry, Mainz, Germany, [2]Johannes Gutenberg University, Institute for Atmospheric Physics, Mainz, Germany, [3]Max Planck Institute for Chemistry, Particle Chemistry Department, Mainz, Germany

Within high altitude clouds and the fully glaciated part of deep convective clouds ice crystals grow predominately under supersaturation by diffusion i.e., the deposition of water vapor into the solid phase. Trace atmospheric constituents such as volatile organic compounds (VOCs) may co-deposit into the crystal structure during growth possibly being transported from the boundary layer into the upper troposphere. This co-deposition process is quantified by gas-ice partitioning coefficients. Once in the ice phase, the VOC constituents may be vertically redistributed by scavenging and subsequent precipitation or by sublimation of these ice crystals at high altitudes. This vertical distribution is critical for the chemical species' role in a host of important atmospheric processes such as secondary organic aerosol (SOA) creation, cloud formation, and subsequent radiative forcing.[1–3] This work presents a method to experimentally determine gas-ice partitioning coefficients for a variety of potential SOA precursors and the calculated coefficients for a series of relevant carbonyl SOA precursors, e.g. benzaldehyde, nopinone, methyl vinyl ketone. Gas-ice partitioning coefficients are calculated by the relative concentrations of a constituent in the gas phase and the deposited ice phase. Here these concentrations are measured in a flowtube type apparatus under simulated atmospheric conditions in temperatures ranging from -40°C to -80°C. Gas phase measurements are collected using an annular denuder method with an in-situ derivation as described by Kahnt et al. 2011.[4] Both the gas phase denuder extract and ice phase concentration are quantitated using reverse phase HPLC with a solid phase extraction preconcentration.

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3) Liu et al. *Geophys. Res. Lett.* **2018**, *45* (9), 4410–4418. https://doi.org/10.1029/2018GL077517.

4) Kahnt et al. *J. Chromatogr. B Anal. Technol. Biomed. Life Sci.* **2011**, *879* (17–18), 1402–1411.

Revealing the interfacial dynamics between antifreeze proteins and the ice-water interface at single-molecule level through subzero nanoscopy

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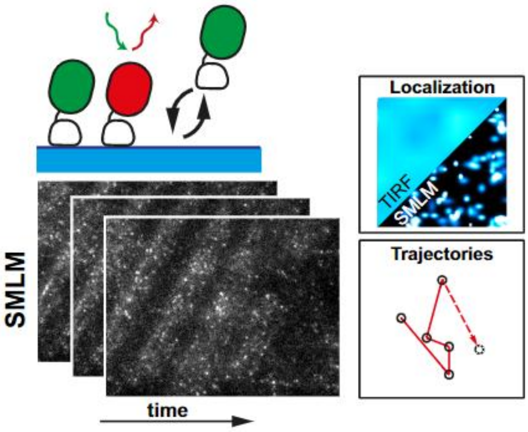
Department of Chemical Engineering and Chemistry, Laboratory of Self-Organizing Soft Matter, Eindhoven University of Technology, Eindhoven 5612 AP, the Netherlands; and Institute for Complex Molecular Systems, Eindhoven University of Technology, Eindhoven 5612 AP, the Netherlands



Fig(1) Single-molecule localizations of AFPs at the ice-water interface by extracting the position (Top) and dynamics (Bottom) with diffraction-unlimited resolution [2].

Antifreeze proteins (AFPs) are unique proteins that bind to growing ice crystals, and thereby reduce the freezing temperature, thermal hysteresis, and/or inhibit ice recrystallization. Cold-blooded organisms produce these proteins to endure the extreme cold of their natural habitat[1]. Although AFPs have been investigated over 50 years, the interfacial dynamics involved during binding remain uncertain. To bridge this gap, our group designed a subzero nanoscopy set-up to investigate AFPs on a single-molecule level. Recently, this technique revealed that irreversible pinning is required for thermal hysteresis but not for ice recrystallization inhibition[2]. In this presentation, I will explain how our group studied the underlying mechanism at the ice-water interface.

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2) Tas, R. P., Hendrix, M. M. R. M. & Voets, I. K.. *Proc Natl Acad Sci U S A* **120**, e2212456120 (2023).

7-A1-1 9：00-9：20

Hydrogen-ordered states of ice V-XIII revisited: β-state between the two

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Water ice has tremendous structural variety even for the mono-molecular system. In addition to the O-atom network diversity, different configurations for orientations of H_2O molecules enrich ice polymorphism, currently counting to twenty. Ice V is a disordered high-pressure phase stable at 0.3–0.6 GPa below 270 K. This phase takes at least two pathways of hydrogen ordering at 105–120 K upon cooling [1], which are not understood.

Here, we re-examine the hydrogen-ordering process to ice XIII at ambient pressure using differential scanning calorimetry (DSC). HCl-doped ice V was annealed isothermally for 40 min at different temperatures between 93–129 K, where point defect doping facilitates hydrogen ordering [1]. Figure 1 summarises the temperature dependence of enthalpy release, ΔH, and the peak temperature, $T_{\max}$ for hydrogen disordering. Below 110 K, ΔH (and hence the degree of H-order) increases with temperature while $T_{\max}$ remains at ~120 K, suggesting that hydrogen ordering proceeds faster at higher temperatures but reaches the same ordered state, ice XIII. Above 110 K, $T_{\max}$ increases and has a maximum at 114 K while ΔH monotonically decreases. These trends imply a different (but unknown) ordered state, which we call the β-state, distinct from both ices V and XIII in an H-order manner. Further details will be discussed in the presentation with comprehensive observations.

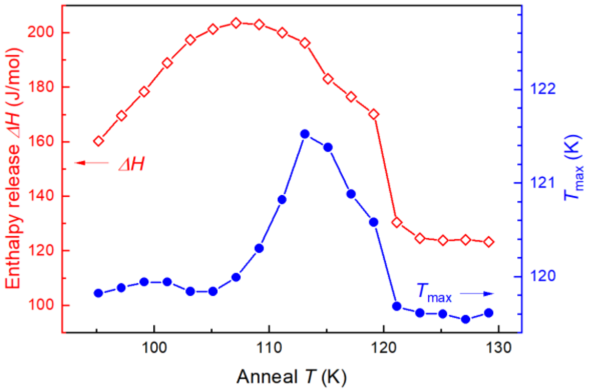

Figure 1 Characteristic values of ice XIII disordering endotherm observed upon heating at 30 K/min after annealing of ice V at T (K) for 40 min. Red open diamonds and blue solid circles correspond to enthalpy release ΔH (left) and peak temperature $T_{\max}$ (right), respectively. Colours are available in pdf version.

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7-A1-2 9:20-9:40

Is a hydrogen-ordered phase corresponding to ice IV experimentally accessible?

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Geochemical Research Center, Graduate School of Science, the University of Tokyo. 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan.

Ice IV is a metastable high-pressure phase of ice, whose hydrogen-atom sublattice has a disordered structure in the time-space averaged crystal structure[1]. However, the hydrogen-ordered counterpart of ice IV is missing to date. According to previous studies by Salzmann and coworkers, HCl-doped ice IV samples quench-recovered to ambient pressure under liquid nitrogen show a weak endotherm during heating in differential scanning calorimetry (DSC) measurements[2,3]. This indicates the presence of *a low-temperature state* related to ice IV, perhaps its partially hydrogen-ordered counterpart, but the origin of the endotherm remains unclear to date. For example, this endotherm may be also explained by unfreezing the orientational glass.

To address this issue, we have conducted *in-situ* powder neutron diffraction experiments of ice IV at the high-pressure neutron diffractometer *PLANET* in J-PARC. When doped ice IV was slowly cooled under pressure, we found a very small but clear $\partial V/\partial T$ discontinuity at low temperatures. In addition, Rietveld refinements of low-temperature diffractograms resulted in a very weakly hydrogen-ordered structure along the c axis. However, its extremely weak degree of hydrogen order, which was also suggested by small ΔS values estimated from the DSC data presented in the previous studies[2], hinders further detailed discussions regarding its low-temperature ground state(s) and the assignment of a new Roman numeral to this “low-temperature phase” with confidence. In the presentation, potential strategies to enhance the degree of ordering will be also discussed.

[1] H. Engelhardt and B. Kamb, J. Chem. Phys. **75**, 5887 (1981).

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[3] C.G. Salzmann, P.G. Radaelli, B. Slater, and J.L. Finney, Phys. Chem. Chem. Phys. **13**, 18468 (2011).

Ice XIX: The second hydrogen-ordered daughter phase of ice VI

Tobias M. Gasser[1], Alexander V. Thoeny[1], Thomas Loerting[1]

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Order is the most important characteristic of crystal structures. This also applies to crystalline H_2O ice. Nevertheless, a distinction is made between ordered and disordered ice phases. While O atoms in the lattice show translational order, this is not always true for H atoms. In fact, the H atom lattice of hexagonal ice and in six high-pressure ice poymorphs is not ordered. Yet, an ordered counterpart is known for all these ice phases (except ice IV). Ice VI and its ordered daughter ice XV [1] represent a special case. In 2018, calorimetry measurements have revealed an intriguing endothermic feature about 25 K below the XV→VI phase transition [2]. Together with XRD, Raman and dielectric spectroscopy findings this has proven the existence of a second, hydrogen-ordered daughter phase of ice VI, ice XIX [2]. Neutron diffraction measurements reveal ice XIX to be ordered antiferroelectrically and to crystallize in a $\sqrt{2} * \sqrt{2} * 1$ supercell of the ice VI unit cell. Out of 2000 possible structural models the powder data fit best a $P\bar{4}$ model [3,4]. Recently, a different structure was proposed for ice XIX [5]. However, the sample used in this study is lacking the catalyst that actually allows the ordering to take place. The disordered and distorted structure suggested in ref. [5] hence represents a pre-cursor state to ice XIX, but cannot be called ice XIX. We suggest to call it ice VI'. Ice XIX represents the first example of a disordered mother phase with two ordered daughters. Yet, ice VI has by no means revealed all its secrets.

1) C.G. Salzmann, P.G. Radaelli, E. Mayer, J.L. Finney, *Phys. Rev. Lett.,* **103**, 105701 (2009)
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3) T.M. Gasser, A.V. Thoeny, A.D. Fortes, T. Loerting, *Nat. Commun.*, **12**, 1128 (2021)
4) R. Yamane, K. Komatsu, J. Gouchi, Y. Uwatoko, S. Machida, T. Hattori, H. Ito, H. Kagi, *Nat. Commun.*, **12**, 1129 (2021)
5) C.G. Salzmann, J.S. Loveday, A. Rosu-Finsen, C.L. Bull, *Nat. Commun.*, **12**, 3162 (2021)

Kinetics of the hydrogen order-to-order transition in ice XV/XIX

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The first case of two distinct types of H-order in a given lattice of O-atoms in H_2O-ice chemistry is ice XV/XIX. These two polymorphs are linked by an H-order-order transition. Hence, ice XV/XIX represents the first example on which both a H-order-order phase transition and the mechanism leading to different kinds of H-order can be studied [1].

Here we study the kinetics of an H-order-order transition based on isothermal waiting experiments using both dielectric spectroscopy and Raman spectroscopy. The latter technique is ideal because the disordered mother phase ice VI and the two ordered daughter ices XV and XIX can be clearly identified and quantified through well-separated marker bands. It turns out that ice XIX transforms in a first step into a transient, disordered state called ice VI‡ before the order in ice XV develops in the second step [2]. We deduce rate constants and activation energies for both steps individually. Isotope substitution experiments reveal a huge effect on the first step, ice XIX decay, but a much smaller effect on the second step, ice XV build-up [2], which is suggestive of quantum tunneling playing an important role only for ice XIX decay. Furthermore, we also reveal impact of H-doping on deuterated ice XIX, where a significant acceleration of D-reorientation dynamics is encountered through H-doping. That is, H-doping represents the *conditio sine qua non* without which D_2O ice XIX cannot be produced (at least on the time scale of months in the laboratory).

1) T. M. Gasser, A. V. Thoeny, A. D. Fortes and T. Loerting, *Nat. Commun.*, **12**, 1128 (2021).
2) 2) A. V. Thoeny, I. S. Parrichini, T. M. Gasser, and T. Loerting, *J. Chem. Phys.,* **156**, 154507 (2022).

7-A2-1 10:40-11:10

The Mechanical Properties of Freshwater Ice

Ian Baker

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In Nature, deformation of ice occurs at over 80% of its melting point. The strength of ice decreases rapidly with increasing temperature and shows a Hall-Petch relationship with the grain size. Based on creep tests, Glen (1955) first developed a flow law for the secondary creep of polycrystalline ice in which the strain rate, $\dot{\varepsilon}$, is related to the stress, s, through $\dot{\varepsilon} = A\sigma^{n}$, where the stress exponent, $n \approx 3$. However, some more recent studies of polycrystalline ice have indicated values of n from 1-4 depending on the temperature and grain size. In contrast, deformation of single crystal ice generally shows $n \approx 2$. Deformation of ice is largely controlled by dislocation glide on the basal plane, which has been suggested to be related to the rate of hydrogen-bond reorientation. The CRSS for non-basal slip is almost two orders of magnitude higher than that for basal slip. Thus, the flow of polycrystalline ice is strongly affected by grain orientation, which changes during deformation both due to slip-plane rotation and to recrystallization, which can occur at strains of a few percent. It is well established that the Earth's large continental ice sheets contain a variety of naturally-occurring impurities, both soluble and insoluble, both of which can have substantial effects on the flow of ice. This presentation will review both the phenomenology and mechanisms of ice deformation with an emphasis on the effects of both soluble impurities and particles.

J.W. Glen, "The creep of polycrystalline ice" Proceedings of the Royal Society of London, **A228** (1955) 519–538. http://doi.org/10.1098/rspa.1955.0066

Ice Creep and Behavior of Ice Borehole

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The creep is one of the most variable properties of ice because it depends on temperature, crystal orientation, dust content, and other factors. Even most glaciologists have adopted Glen's Law, at present, a universal constitutive law for ice creep does not exist. Ice creep has a very strong influence on drilling technology because during underbalanced drilling the borephole will close. Drill sticking is the most severe drilling problem that can occur in ice borehole because of closure. Despite the success in ice-drilling technology, there remain examples of coring accidents not only in warm ice but also in temperate and cold ice. Therefore, the selection of reliable borehole closure prediction has to be considered during the planning stage of all ice-core drilling projects.

Proposed method allows to predict borehole closure both in dry and wet boreholes. The closure of the dry borehole is the most severe. The borehole with near-surface temperature of -20 °C closes quickly, and dry drilling can safely be accomplished to a depth of ~230 m only. In contrast, a borehole with a near-surface temperature of -50 °C can be drilled without potential accidents to a depth close to 500 m.

For drilling at greater depth, it is necessary to prevent closure by filling the borehole with a fluid. However, it is impossible to prevent borehole closure at all, because in any case there will be parts in the borehole where the ice pressure is more than the pressure of fluid. That is why, after selection of the drilling fluid, potential borehole closure should be estimated. Recently, synthetic-based drilling fluids based on the aliphatic synthetic ester ESTISOL™ 140 is considered as the most appropriate non-freezing fluid for drilling in Antarctica. Our estimations of borehole closure for SPICEcore borehole at the South Pole drilled with ESTISOL™ 140 have very good correlation with the recent borehole observations using acoustic televiewer. The proposed method allows one to choose the correct column of drilling fluid and fluid density for the concrete drilling site.

7-A2-3 11:30-11:50

Ice of H2O with some additives: Experimental observations on mechanical properties

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Pure H2O, when frozen without sophisticated process, leads to poor mechanical properties of H2O ice, lower than mechanical properties of classical natural hailstones. In order to mimic mechanical properties of hailstones, we tested several additives to H2O. Here we present the main observations.

In particular, we present the maximum shear stress of an ethanol/ H2O mixture on stainless steel, as a function of temperature. We experimentally observe changes in behavior at temperatures previously identified as transition temperatures between different ethanol hydrates [1].

We also present other additives we tested, that enhanced or lowered the mechanical behavior: red wine vinegar, acetic acid, sodium bicarbonate, glycol, hydrogen peroxide, and acetone.

1) Facq, S., Danède, F., & Chazallon, B. *The Journal of Physical Chemistry A*, 117(23), 4916–4927(2013)

What controls crystallographic preferred orientations (fabrics) of deformed ice: constraints from laboratory experiments

David J. Prior[1], Chao Qi[2], Lisa Craw[3], Andrew Cross[4], S. Fan[1], David L. Goldsby[5],
Travis Hager[5], Qinyu Wang[2],.

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Crystallographic preferred orientations (CPOs commonly called fabrics in the glaciological literature) develop in polycrystalline ice as a result of deformation and dynamic recrystallisation. Strong CPOs are ubiquitous in the ice that makes up Earth’s glaciers and ice sheets and give rise to significant mechanical anisotropy that needs be incorporated into ice sheet flow models. Laboratory experiments provide some of the best constraints on how CPOs correspond to deformation kinematics and conditions and give insights into the micro-scale mechanisms that control CPO development. Modelling needs to predict the CPO that forms, and how stable it will be if deformation kinematics or conditions change.

Some interpretations of CPOs in ice cores are inconsistent with the empirical results of laboratory experiments. The most significant example is the strong vertical *c*-axis maximum observed in many ice cores from ice divides and domes, that is often interpreted as the result of vertical compression. A strong *c*-axis maximum parallel to compression cannot be generated in the laboratory. The only experiments that generate single strong *c*-axis maxima are shear experiments, where the maximum lies normal to the shear plane and ~ 45 degrees to the compression axis.

Laboratory experiments give an internally consistent set of results that can be scaled to the slower strain rates of natural deformation. Strong single and double *c*-axis maxima correspond to non-coaxial (rotational) shear, *c*-axis distributed on a small circle (cones) are developed in coaxial flattening. We will outline the mechanistic controls on these CPOs and discuss how to rationalize these data with observations from glaciers and ice sheets.

7-A3-2 13:50-14:10

The Impacts of Impurities and Stress State on Polycrystalline Ice Deformation and Fabric Evolution

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Understanding glacier and ice sheet behavior is crucial for interpreting ice core records and predicting their future impact on sea level rise. While research has been conducted on the physical and mechanical properties of polycrystalline ice, very little has been reported about the effects of soluble impurities on these properties. Variations in impurity concentrations have been associated with variations in deformation rates in both Greenland and Antarctica (Thorsteinsson et al., 1997; Pettit et al., 2007), underscoring the need for further investigation.

Our study aims to quantify the effects of impurities, particularly sulfuric acid on the mechanical behavior and microstructural evolution of polycrystalline ice under uniaxial compression and simple shear. We are conducting experiments on polycrystalline ice samples containing varying interlayings of sulfuric acid, using a combination of mechanical testing, microstructural analysis and microchemical analysis.

Preliminary results suggest that sulfuric acid influences the onset and rate of recrystallization, decreases the strength, and becomes concentrated at the grain boundaries and triple junctions, potentially causing a liquid phase to exist through drag of grain boundaries and lattice sweep in polycrystalline ice under uniaxial compression. The results of this study will provide valuable insights and inform models for layered media about the mechanisms that govern vertical thinning within ice sheets.

1) E. Pettit, T. Thorsteinsson, H. Jacobson, E. Waddington. The role of crystal fabric in flow near an ice divide. *Journal of Glaciology*, *53*(181), 277–288 (2007). https://doi.org/10.3189/172756507782202766

2) T. Thorsteinsson, J. Kipfstuhl, H. Miller. Textures and fabrics in the grip ice core. *Journal of Geophysical Research: Oceans*, *102*(C12), 26583–26599 (1997). https://doi.org/10.1029/97jc00161

7-A3-3 14:10-14:30

Effect of high-pressure sintering on snow density evolution: Experiments and results

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Very few studies have emphasized the effects of high-pressure sintering on snow density evolution, even though snow as a type of engineering material is widely used in construction engineering in cold regions for snow pavement, snow runway and polar infrastructure. This study presents new experimental results of snow densification under high pressures of up to 100 MPa for a temperature range from -3.5 to -17.3 ℃ and uniaxial compression at the temperature of -10 ℃ and constant strain rates from 5×10^{-4} to 10^{-1} s^{-1}. Results reveal that density evolution of snow to ice under high-pressure sintering can be achieved in a wide temperature range within a duration as short as 5 mins. The compressive strength of snow-sintered ice was about 1.2 to 2.2 times as large as that of water-frozen ice reported by previous work. The orthogonal experiment showed that pressure is a more significant factor affecting the final density in comparison with sintering temperature and time. The increased rates of ice fabrication, low limitations on temperature, and reliable sintered snow strength indicate that snow-ice engineering, such as airport construction in Greenland and Antarctica, can be improved by high-pressure sintering of snow to overcome the harsh environment.

7-A3-4 14:30-14:50

Effects of impact heating on porous icy bodies like comets

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Comet nuclei mainly consist of icy materials (H_2O and volatiles). Recent spacecraft explorations have revealed that comet nuclei have high porosity of 40-80% [e.g.1]. When a small body impacts on such a porous icy body at a high velocity, the kinetic energy would deposit efficiently as post-shock heat around the crater. The post-shock heat might be one of the most important heat sources for thermal evolution of porous icy bodies, and it would induce crystallization of amorphous ice around the impact crater. It may also promote evaporation of volatiles, and these volatiles might be stored underground at high pressure. As a result, they could push against and break the surface crust. In this study, we studied the post shock heating around the crater on porous ice based on our in-situ observations of the post-shock heating on porous ice. We then discussed the areas where amorphous H_2O ice would crystallize and volatiles would be depleted on comet nuclei.

We conducted impact experiments on porous H_2O ice target with the porosity of 40-60% by using two-stage light gas gun installed in a cold room at -15ºC. The impact velocity was 3-6 km/s. Projectiles were aluminum sphere with the diameter of 2mm. The temperature inside the target was measured by several thermocouples and the maximum temperature distribution was obtained. From this temperature distribution, the energy partition coefficient from projectile kinetic energy to post shock heat was estimated to be 8-60% depending on target porosity and impact velocity.

Post-shock heat on porous icy body was calculated numerically using a heat conduction model assuming that the post shock heat was calculated by using the energy partition coefficient and was initially embedded into the thin liquid-ice water layer on the crater wall. As a result, the volatile depletion zone on comet nuclei expanded with the increase of initial temperature of comet surface although it was confined around the crater and was smaller than one crater radius from the crater wall. The crystallization zone expanded with the increase of initial temperature of comet surface and the increase of crater radius. But the crystallization zone also only appeared close to the crater wall as well as volatile depletion zone.

1) Pätzold et al., *Nature*, **539**, 63–65 (2016).

7-A4-1 15:10-15:30

Ice multiplication associated with freezing of supercooled water droplets

Alexei Kiselev[1], Amelie Assenbaum[2], Alice Keinert[1] and Thomas Leisner[1]

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More than 6 decades after the seminal works of Mason and Maybank in 1960 [1], Dye and Hobbs in 1966 [2], Takahashi and Yamashita in 1970 [3], and many others, we are still struggling to fully understand the process of ice multiplication accompanying freezing of freely falling water drops. This mechanism, however, is thought to contribute considerably to the process of ice multiplication in atmospheric clouds and is, therefore, of utmost importance for correct modelling of aerosol-cloud interactions and precipitation formation. In this contribution we report on the recent advances in observation of droplets freezing and fragmentation obtained in our group using a combination of electrodynamic levitation, high speed video observations and IR thermography [4-6]. We show how the IR temperature measurements of the freezing droplet allow detecting the pressure rise and fall inside the freezing drop and how the pressure release events are correlated with the various types of droplet splintering revealed by the high-speed video microscopy. Finally, we report on the most recent experiments performed with the capillary-suspended droplets and analyze the freezing behavior characteristic for the various temperature range and flow conditions. The results are interpreted in terms of mechanical properties of ice and ice growth conditions.

1) Mason, B.J. and J. Maybank, QJRMS, 1960. 86(368): p. 176-185.
2) Dye, J.E. and P.V. Hobbs, Nature, 1966. 209: p. 464 - 466.
3) Takahashi, C. and A. Yamashita, Journal of the Meteorological Society of Japan. Ser. II, 1970. 48(4): p. 373-376.
4) Kleinheins, J., A. Kiselev, A. Keinert, M. Kind and T. Leisner, JAS, 2021, 78, 1703.
5) Keinert, A., D. Spannagel, T. Leisner and A. Kiselev, JAS, 2020, 77, 2959-2967.
6) Lauber, A., A. Kiselev, T. Pander, P. V. K. Handmann and T. Leisner, JAS, 2018, 75, 2815-2826.

7-A4-2 15:30-15:50

Dielectric-Infrared Spectrum of Ice and Atomic Dynamics Behind It

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Distinctions between ice and water determine processes of various scales from the adaptation of living organisms to the formation of planets. In this talk, I will critically review ice's dielectric response from direct current to infrared (Fig.1). The corresponding molecular and protonic dynamics will be discussed in fine detail and compared with that of liquid water. I will provide microscopic interpretation for such curious facts as the close dielectric constant of ice and water, higher protonic conductivity of ice compared to water in the megahertz region, and anomalously stable vibrational terahertz mode. The differences between ice and water will be described within a universal microscopic model [2]. The new approach simplifies the modeling of the spectra from DC to the infrared and provides new insights into the structure and dynamics of ice and water.

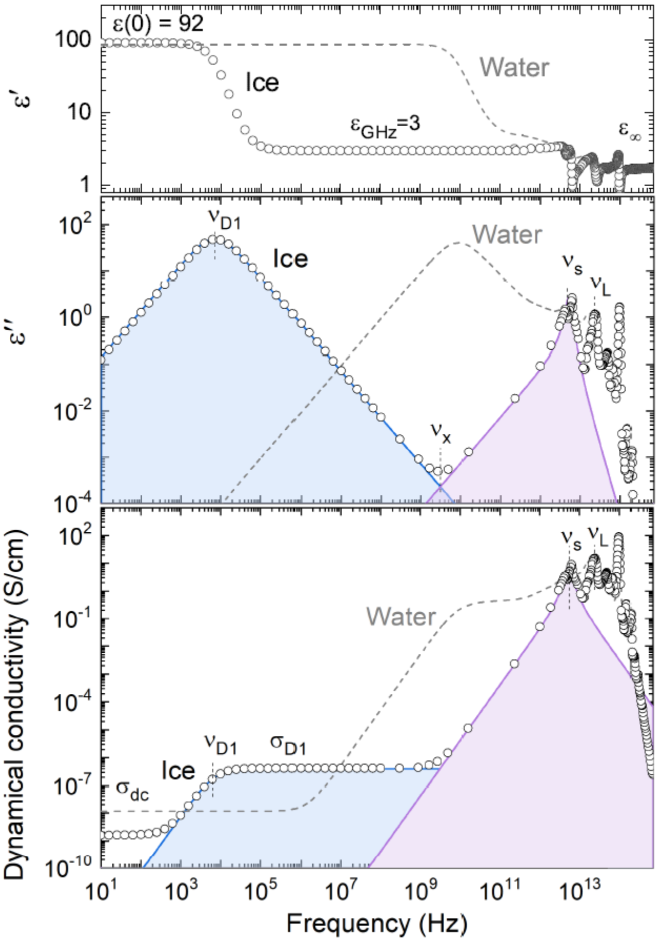

Figure 1: The broadband spectra of ice and water near melting point in terms of real (top) and imaginary (middle) parts of the dielectric permittivity, and dynamic conductivity (bottom) [1].

[1] V. Artemov, “The Electrodynamics of Water and Ice”, Springer (2021).
[2] V. Artemov, A unified mechanism for ice and water electrical conductivity from direct current to terahertz, *Phys. Chem. Chem. Phys.*, **21**, 8067–8072 (2019).

7-B2-1 10:40-11:10

Analysis of Antifreeze Proteins from Japanese Organisms

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We have been explored antifreeze proteins (AFPs) from Japanese fishes, insects, and fungi. Their DNA sequence, amino acid sequence, biochemical property, ice-binding function, crystal structure, and cell-preservation ability were clarified for each AFP species. Numbers of fishes living in Japan, some of which are available in general food markets, contain type I－III AFPs (AFP I－III) and antifreeze glycoprotein (AFGP) (Fig. 1). Such discovery first demonstrated that AFPs and AFGP are not special proteins for organisms in polar area, but are widely distributed in the middle latitudes covering Asian countries [1]. Activity-modified mutants of AFP III were synthesized to determine their crystal structures, which revealed that the strongest mutant accompanies “ice-like” water network on its ice-binding site. An observation that several waters in this network showed complementary position-match with the waters constructing a single ice crystal allowed us to hypothesize ice-binding model of AFP that utilizes the ice-like water network [2]. On the basis of such findings, technological developments to control water freezing are now progressed in both industry and medical fields.

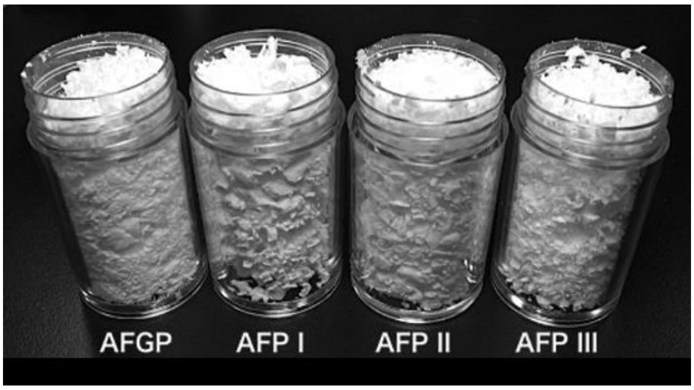

Figure 1. AFP samples (~0.5g) prepared from Japanese fishes.

References

1) S. Mahatabuddin, S. Tsuda: *Adv. Exp. Med. Biol.*, 1081, 321-327 (2018). doi: 10.1007/978-981-13-1244-1_17.

2) S. Mahatabuddin, D. Fukami, T. Arai, Y. Nishimiya, R. Shimizu, C. Shibazaki, H. Kondo, M. Adachi, S. Tsuda: *Proc. Natl. Acad. Sci.* USA, 115 (21), 5456-5461 (2018) doi: 10.1073/pnas.1800635115.

Ice-cold and crystal-clear: pinning and surfing of ice-bound antifreeze proteins imaged one by one with subzero nanoscopy

Roderick Tas, Tim Hogervorst, Sanne Giezen, Daniëlle van den Broek, Romá Surís-Valls, Ilja Voets[1]

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In this talk I will present highlights of recent work[1] on ice-binding proteins (IBPs) and bio-inspired, engineered ice-binding materials.[2] We study how and why IBPs bind ice crystals using single molecule experiments (nanoscopy) and relate adsorption behavior to their activity[3] aiming to achieve a solid mechanistic understanding of how IBPs work and as a stepping stone towards the knowledge-based design of synthetic (ice) crystal growth modifiers[2] for biomedical and other applications.[4,5]

1. Tas, R. P.; Hendrix, M. M. R. M.; Voets, I. K., Nanoscopy of single antifreeze proteins reveals that reversible ice binding is sufficient for ice recrystallization inhibition but not thermal hysteresis. Proc. Natl. Acad. Sci. 2023, 120 (2), e2212456120.
2. Surís-Valls, R.; Hogervorst, T. P.; Schoenmakers, S. M. C.; Hendrix, M. M. R. M.; Milroy, L.; Voets, I. K., Inhibition of Ice Recrystallization by Nanotube-Forming Cyclic Peptides. Biomacromolecules 2022, 23 (2), 520-529.
3. L. L. C. Olijve, K. Meister, A. L. DeVries, J. G. Duman, G. Shuaiqi, H. J. Bakker, I. K. Voets Proc. Natl. Acad. Sci. 2016, 113, 3740-3745.
4. Voets, I. K., From ice-binding proteins to bio-inspired antifreeze materials. Soft Matter 2017, 13 (28), 4808-4823.
5. Tas, R. P.; Sampaio-Pinto, V.; Wennekes, T.; van Laake, L. W.; Voets, I. K., From the freezer to the clinic. EMBO reports 2021, 22 (3), e52162.

7-B2-3 11:30-11:50

Observation of dynamics of ice-crystals on the surface of antifreeze proteins by using time-resolved X-ray diffraction analysis

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Antifreeze proteins (AFPs) are ice-growth inhibitors, which bind to specific planes of a hexagonal ice-crystal[1]. Since the binding of AFPs is mediated by ice-like hydration water on their surface, dynamics of such frozen hydration water is important to understand the ice-binding mechanism. However, there is no report about the real-time observation of dynamics of ice-like water on the AFP surface. Here, we observed the dynamics of frozen-hydration water on the surface of fish-derived AFPs by using the time-resolved X-ray diffraction with the diffracted X-ray blinking method[2]. This new technique estimates the dynamics of crystalline objects by monitoring the intensity fluctuations of their X-ray diffraction. In the current study, AFP powder was irradiated with an X-ray beam below 0°C and its diffraction was recorded with a time interval of 50 ms. The intensity fluctuation was analyzed with autocorrelation function, and it was fitted with a single exponential curve to obtain decay constant, which is an indicator of crystal motion. The X-ray diffraction images showed that ice-crystals on the AFP were rearranged during the measurement and their structures are highly mobile at −30°C but not at −80°C. On the other hand, such motion was not observed in a control protein bovine serum albumin. These results suggest that such “flexible ice-crystals” may be important for the ice-binding function of AFPs.

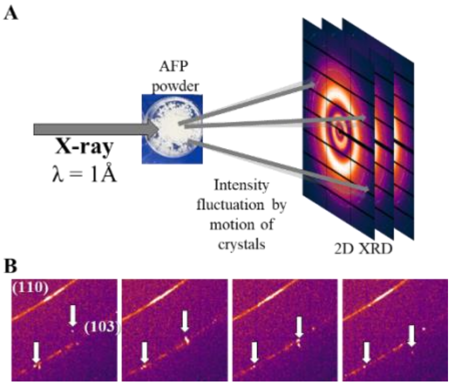

Fig. (A) Experimental setup. (B) Movement of diffraction spots, indicating rearrangement of the ice-crystal lattice.

1) DeVries, A. L. & Wohlschlag, D. E. *Science (80-.)*. **163**, 1073–1075 (1969).
2) Sekiguchi, H. et al. *Sci. Rep*. 8, 17090 (2018).

7-B3-1 13:30-13:50

Monitoring Ice Growth in Aqueous Solutions with Atomic Force Microscopy in the Presence of Ice-Binding Proteins

Ido Braslavsky[1], Michael Chasnitsky[1], Daniel Waiger[1], Ron Tzur[1], Naomi Gillis[1], Yinon Rudich[2], Sidney R. Cohen[3]

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Ice-binding proteins (IBPs) are promising candidates for applications in tissue preservation and food processing, as they have been shown to lower the freezing point and inhibit crystal growth effectively [1]. However, the microscopic mechanisms of IBP action remain incompletely understood, and further insights into their action could be gained through enhanced imaging capabilities. We present a new system design for dynamic atomic force microscopy (AFM) cryo-stage, enabling the study of ice covered with IBPs within a supercooled solution [2]. By imaging the growing ice crystals at the tens of nm scale, we observed characteristic structures rationalized by selective inhibition, which will be discussed in relation to previous, lower-resolution optical images. Overcoming challenges such as moderating and controlling heating, preventing cantilever freezing, and monitoring the boundary between liquid and solid was crucial for achieving these results. Our new set-up enabled control of ice growth in the presence of IBPs and demonstrated the feasibility of measuring less-controlled ice growth in the absence of IBPs. We observed small pits near the apex of growing tapered structures, which can be understood in light of the attachment of IBPs to specific planes. This study suggests the feasibility of investigating particle engulfment at high resolution and measuring the mechanical properties of surface-adhered cells in a partially frozen environment, thus opening new avenues in cryobiology.

1) M. Bar Dolev, I. Braslavsky, P.L. Davies, , *Annu. Rev. Biochem.* **85**, 515–542 (2016).
2) M. Chasnitsky, S. R. Cohen, Y. Rudich, I. Braslavsky, *J. Crys. Growth,* **601**, 126961 (2023)

7-B3-2 13:50-14:10

Ice-binding proteins for cryopreservation

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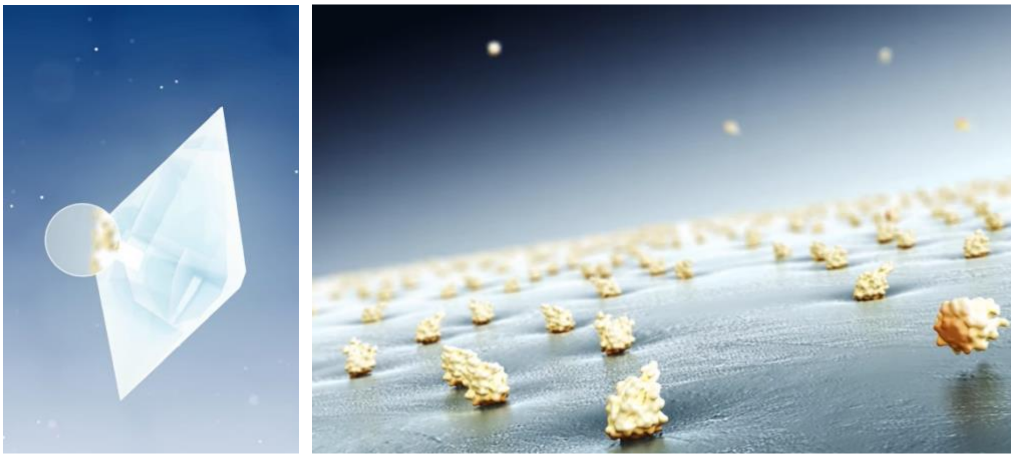
In organisms that inhabit extremely cold environments, ice-binding proteins (IBPs) are vital to prevent freezing damage. Through these proteins, nature may provide inspiration to solve issues of freezing damage in our society. In the medical world, IBPs could enable the long-term storage of biological materials in frozen condition (cryopreservation), for example urgently needed donor hearts.[1] IBPs generally modulate ice crystal size and shape, but portray a remarkably large variety in structure and ice-binding activity among different organisms: some depress the freezing point (thermal hysteresis), while others inhibit the recrystallization process or promote ice nucleation. We systematically study natural IBPs and modified versions, to elucidate how the protein structure is related to the different aspects of ice-binding activity and to the binding dynamics at the ice-water interface. Ultimately, we will apply these insights to rationally engineer IBPs that are optimized for cryopreservation.



1. Tas, R. P., Sampaio-Pinto, V., Wennekes, T., Laake, L. W. & Voets, I. K. From the freezer to the clinic. *EMBO Rep.* **22**, (2021).

Effect of dehydration on cryopreservation process using aquaporin4-overexpressing cells

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Cryopreservation of cells has been used for industrial applications such as breeding and species preservation and is also expected to be used in medicine. The widely accepted concept of cryopreservation is that the dehydration during freezing prevents the formation of ice crystals in the cell [1]. However, there are many cell types that cannot be cryopreserved using current technology, which indicates that the mechanism of cryopreservation, including the dehydration process, has not been fully elucidated. In this study, we investigated the effect of the dehydration process on cryopreservation.

To reveal the effects of dehydration on the cryopreservation processes, we used a unique cell line: Chinese hamster ovary (CHO-K1) cells overexpressing aquaporin4 (AQP4) genetically in plasma membrane. AQP4 is a water channel protein that increases the water permeability of cell membranes. Since the dehydration is induced by the freezing of extracellular water, we compared the cell viabilities at various cooling rates. We also used two cryoprotectants (CPAs), which are used to improve viability in cryopreservation. One is the membrane-permeable CPA, dimethyl sulfoxide (DMSO), which is widely used in the current technology, and the other is the impermeable CPA, trehalose which is a candidate of natural CPAs. These CPAs are expected to induce different osmotic pressures during cryopreservation.

Cells were frozen at cooling rates from 1 to 200 K/min, and viability was measured after quick thawing. The result indicated that cells frozen at less than 80 K/min had higher viability with DMSO, regardless of AQP4 overexpression. On the other hand, the viability of AQP4-overexpressing cells was higher than that of normal cells at more than 80 K/min, regardless of the type of CPAs. This means that the effect of the dehydration process changed depending on the cooling rate.

1) P. Mazur, “Freezing of living cells: mechanisms and implications”, *Am J. Physiol.-Cell Physiol.,* **247**, C125-C142 (1984)

7-B3-4 14:30-14:50

Cryopreservation of trehalose-transporter expressing cells adhered on glass

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In recent years, researches using cells have been attracting attentions as an alternative technology of those using animals. Therefore, the cryopreserving cells has become important technology to supply the necessary cells on demand. Cell cryopreservation is a technique that has already been used in the livestock and fishery industries. Usually, cryopreserved cells are dispersed in a frozen solution. So, it is necessary to culture the thawed cells before using them for testing, which requires undesirable time and efforts and requires facilities. To omit this process, in this study, we aimed to develop a technique for cryopreserving cells in an adherent state.

In general, the cell in an adherent state is more difficult to cryopreserve than in a dispersed state because the damages caused by ice crystals during freezing are greater. We have studied the disaccharide trehalose as a cryoprotective agent (CPA) with unique cells expressing the trehalose transporter (TRET1) to incorporate trehalose into cells. The cells including about 0.5 M trehalose in the dispersed state are confirmed to have high viability [1]. Based on this knowledge, the cells adhere to cover slips were frozen at different temperature from 80°C to -20°C with a small amount of frozen solution including various concentrations of trehalose. After a certain period of storage time (less than one week), the cells were rapidly thawed, and the cell viability was measured by a staining method. As a result, the viabilities of cells without TRET1-expression, which cannot transport trehalose into the cells, was almost 0% at any temperature, but the TRET1-expressing cells had high viabilities at a concentration of about 0.25 to 0.5 M, similar to the dispersed cells. Therefore, it was confirmed that cryopreservation using trehalose is possible even in the adhesive state when the trehalose exists in both intra- and intercellular conditions.

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8-B1-1 9:00-9:30

The Most Potent Snow Makers

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The crystallization of water in clouds plays a key role in weather and climate through its effect on albedo and precipitation. The unassisted, homogeneous nucleation of ice occurs at temperatures lower than -32^{o}C, which are only achieved in high altitude clouds. Ice formation in lower lying, warmer clouds is promoted by atmospheric aerosols. Although the majority of atmospheric aerosols are minerals, the most efficient at forming ice are of biological origin. Ice nucleating bacteria are the most potent ice-nucleating agents in the biosphere and the atmosphere, contributing to cloud glaciation and precipitation, and routinely used for the synthetic production of snow. These bacteria have proteins in their outer membrane that are able to nucleate ice at temperatures as high as -1oC. This presentation will discuss our quest to elucidate the molecular mechanisms by which bacterial proteins and other potent ice nucleants promote water crystallization, what makes them so outstanding, and whether we can design materials that outperform them.

The balance principle on the hydrogen bond network of ice

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In hydrogen-disordered ice, the “ice rule”, in which one water molecule accepts two hydrogen bonds and donates two, is satisfied. In graph theory terms, this describes the *topological* property that the hydrogen-bond network of ice is a regular digraph of degree 2+2. It is also well known that in hydrogen-disordered ice, the orientation of the molecules is random, which gives rise to residual entropy. Hydrogen bonds can be regarded as dipoles. Random molecular orientation leads to random dipole arrangements, which are reflected in the physical properties. This is a *geometric* property. Thus in ice, topology, geometry, and physical properties are deeply connected: It was shown that the convergence of the Kirkwood correlation coefficient for hydrogen-disordered ice satisfying the ice rule is very slow and that some long-range orientational correlation exists, but the mechanism has not been elucidated yet.[1]

We propose a *balance principle* that dominates the structure and property of ice. Based on the principle, it is possible to provide rational explanations for various ice properties, such as why apparent long-range orientational correlations occur in ice and why Pauling was able to accurately estimate the residual entropy with a simple model.[2]

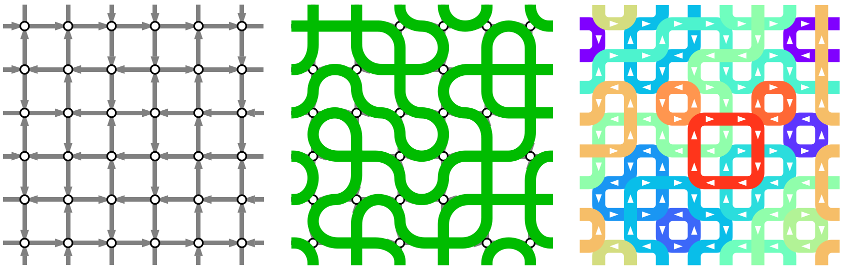

Figure: A digraph of ice, Euler path, and tiling by cycles.

1) F. H. Stillinger, M. A. Cotter, *J. Chem. Phys.* **58**, 2532–2541 (1973).
2) M. Matsumoto, T. Yagasaki, H. Tanaka, *J. Chem. Phys.* **155**, 164502 (2021).

8-B1-3 9:50-10:10

Confinement effects on the o-H_2O↔p-H_2O nuclear spin isomers interconversion mechanism and rates

Patrick Ayotte[1], Thomas Putaud[1,2], Pierre-Alexandre Turgeon[1], Clément Wespiser[1], Jean-Claude Chartrand[1], Jonathan Vermette[1], Yulia Kalugina[1,3], Pierre-Nicholas Roy[3], Xavier Michaud[2]

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At the low temperatures and small number densities typical of the interstellar medium, the interconversion of the water molecule nuclear spin isomers (NSI), o-H_2O↔p-H_2O, is essentially forbidden. However, it occurs readily under confinement at temperatures as low as 4K in inert matrices, as well as within endofullerenes, as revealed by rovibrational spectroscopy. The dependencies of the interconversion effective first-order rate constant (k_{eff}), as well as of the equilibrium constant (the ortho-to-para ratio, or OPR), on the temperature (T = 4K - 30K), on the water molecules isotope ($H_2{}^AO$, A = 16,17, and 18) as well as on the confinement media (rare gases, C_{60}) will be reported [1]. A simple confined rotor model will be shown to provide an accurate description of rovibrational spectra for confined water revealing the topological features of the confinement potential that govern the couplings between the rotational and translational degrees of freedom and that are responsible for the mixing between ro-translational states thereby opening new interconversion pathways that are forbidden in the isolated molecule [2]. Improving our understanding of confinement effect on the NSI interconversion mechanisms and rates should enable better storage strategies [3] to be devised for water samples highly enriched [4] in o-H_2O en route towards surface NMR as well as interfacial chemical dynamics studies. It may also provide more robust interpretations of the NSI populations observed in the interstellar medium.

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8-B2-1 10:30-10:50

Fast crystal growth of ice VII owing to the decoupling of translational and rotational ordering

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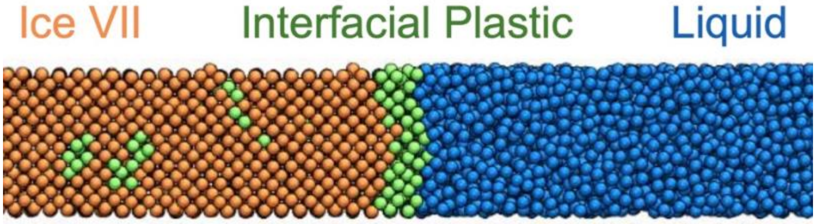
Despite the abundance of water's crystalline polymorphs, the growth mechanisms of most ice forms remain poorly understood. This study applies extensive molecular dynamics simulations to examine the growth of ice VII, revealing a fast growth rate comparable to pure metals while maintaining robust hydrogen-bond networks. The results from an unsupervised machine learning applied to identify local structure suggest that the surface of ice VII consistently exhibits a body-centered cubic plastic ice layer with decoupled translational and rotational orderings. The study also uncovers the ultrafast growth rate of pure plastic ice, indicating that orientational disorder in the crystal structure may be associated with faster kinetics. Additionally, we discuss the impacts of interfacial plastic layer width and surface roughness on growth mode.[1]

1) K. Mochizuki et al, "Fast crystal growth of ice VII owing to the decoupling of translational and rotational ordering", under review



8-B2-2 10:50-11:10

Surface premelting of ice I_c using molecular dynamics simulation

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Surface premelting is a phenomenon in which quasi-liquid layers form on the surface of ice at temperatures below its melting point. This contributes to the remarkably slippery surface of ice and its tribological properties. At the molecular level, tribological phenomena can be interpreted as the diffusion of molecules. Therefore, understanding the molecular origin of ice premelting is of great importance to the tribology industry.

Molecular dynamics simulations have been widely used to study the structural and dynamical properties of ice using both all-atom models and coarse-grained models. In hexagonal ice (I_h), the premelting layers include solid-like and liquid-like regions with sizes up to a few nanometers [1]. The diffusion coefficients have been found to decrease exponentially with decreasing temperature [2]. The basal, first prism, and second prism surfaces demonstrate variations in the ratio of the solid-like and liquid-like regions, as well as in the diffusion coefficients [2]. These studies suggest that surface geometry affects ice premelting. However, the structural and dynamical properties of premelting in ice crystals with different geometries remains unclear.

In this study, we investigate ice premelting in cubic ice (I_c) to compare the dynamics of ice I_c with those of ice I_h, as well as with those of bulk liquid and solid ice. We perform molecular dynamics simulations of the ice-vapor equilibrium of I_c crystals and analyze the molecular trajectories using a novel machine learning technique for water dynamics.

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[2] T. Kling, F. Kling, and D. Donadio, *J. Phys. Chem. C*, (2018), **122**, 24780-24787.

Pore-scale modeling of wet snow metamorphism

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Snow is a porous material composed of two components, water and air, distributed amongst three phases: solid ice, liquid water and air with water vapor. Temperature gradient actively drives phase changes within the snowpack, leading to snow metamorphism. This process could drastically change the hydraulic properties of snowpack and impact meltwater infiltration. However, mechanistic modeling of snow metamorphism remains a key challenge in snow hydrology.

Based on whether liquid water is present, snow metamorphism is considered in two types---dry and wet. In this work, we focus on wet snow metamorphism, which occurs when temperature is close to the melting point. We propose a phase-field model for wet snow metamorphism at the pore scale. The model leverages the phase-field formulation [1] to track the temperature evolution amongst the three phases and the water vapor concentration in the air. This allows us to simultaneously capture three relevant phase-change phenomena: sublimation (deposition), evaporation (condensation), and melting (solidification). Compared to previous models of dry snow metamorphism [2], our model incorporates the liquid water thermodynamics at the pore scale and can be readily extended to incorporate two-phase flow under drainage.

We simulate controlled melting of snow in 2D using a simplified geometry and unveil the impact of vapor concentration on the melting process. We also simulate dry and wet snow metamorphism in a 2D simplified geometry and provide insight into the differences between these two processes in terms of grain size evolution. In addition to wet snow metamorphism of real snowpack, our pore-scale model can investigate other scenarios involving water phase transitions such as a water droplet freezing on a substrate [3].

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2) T.U. Kaempfer, M. Plapp, *Phys. Rev. E*, **79(**3), 031502 (2009).
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Poster Presentations

P-01

Temperature-dependent dissociation degree of nitric acid at the air-ice interface linked to the hydrogen-bonding structure of the ice

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The polar cryosphere is an active medium affecting the atmosphere significantly by exchanging reactive trace gases with the boundary layer. Nitric acid (HNO_3) is formed in the transformation reactions of NOx and removed from the troposphere by wet and dry deposition to surfaces like ice. Open questions remain for the fate of HNO_3 upon adsorption to the ice at the air-ice interface under tropospheric conditions; more specifically, the dissociation degree of HNO_3 and hydrogen-bonding network around HNO_3 depending on the temperature of the ice, as well the products of HNO_3 upon photolysis at the air-ice interface. This research addresses the understudied concept of interfacial acid-base chemistry, next to the environmental importance of the interaction of HNO_3 with ice. Acidic adsorbates on ice have been shown to exist in molecular and ionic forms. The current hypothesis is that the flexibility in the hydrogen-bonding network structure at the air-ice interface drives the dissociation. We investigated the dissociation degree of HNO_3 adsorbed to ice at low coverages using X-ray photoelectron spectroscopy (XPS) at the Swiss Light Source of the Paul Scherrer Institute. We found 84% dissociation of HNO_3 on ice at -30°C, and only 32% dissociation at -50°C. Using oxygen K-edge near-edge X-ray absorption fine structure (NEXAFS) spectroscopy, we probed the changes to the structure of the hydrogen-bonding network upon adsorption of HNO_3 to the ice. Overall, all NEXAFS spectra of the ice remained quite ice-like, independent of the adsorption of HNO_3 to the ice. At -30°C we saw a higher contribution of water molecules that are in an environment similar to aqueous nitrate solutions for ice doped with nitrate than for pure ice, which goes in line with the findings of Křepelová et al. (2010). However, these changes were not observed for ice at -50°C upon dosing HNO_3. This points towards a lower flexibility of the hydrogen-bonding network of the nitrate-doped ice at -50°C than at -30°C, and might be an explanation for the significantly lower dissociation degree of HNO_3 observed for -50°C ice than for -30°C ice.

P-02

Interactions of Small Molecules with the Growth Fronts of Ice Crystal Faces

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Single crystals of hexagonal ice are grown with slow, equilibrium growth in a modified Bridgman apparatus [1]. This method results in thermodynamic growth as the growth crucible is slowly lowered through a temperature gradient to grow the single crystal. Cross section etches reveal orientation of the ice crystal at the growth front. To probe the interaction of different molecules at the ice/water interface, aqueous solutions can be used in the growth apparatus instead of neat water.

Poly (vinyl alcohol) (PVA) is a known ice recrystallization inhibitor and is expected to bind to specific faces of ice based on theoretical models [2]; Zirconium acetate is also known to bind to specific faces of ice [3]. When aqueous solutions are grown in the modified Bridgman apparatus, the ice faces seen at the growth front reveal those that are not inhibited by binding. Results from growth with PVA and zirconium acetate solutions will be reported. In addition to probing interactions affecting ice-growth, complementary information on the interaction of ice-binding molecules can be obtained using the surface specific spectroscopy phase-sensitive sum frequency generation.

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P-03

Non-energetic Chemical Pathways of Sulfur Bearing Species with Hydrogen Atoms on Interstellar Ice

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There have been about 30 sulfur (S)-bearing species identified in the interstellar medium (ISM). Since the observed abundance of S-bearing species in the gas phase is lower than the cosmic abundance of S[1], it is often considered that there might be a source of “missing S" on interstellar grains. Based on an assumption that physico-chemical processes of S-bearing species on interstellar ices would be a key to constrain their presence in the ISM. In the present study, we shed light on the behavior of other S-bearing species, carbonyl sulfide (OCS) and methylmercaptan (CH_3SH), via chemical processes without external energies on interstellar ices at low temperatures (typically 10K) using experimental and computational methods.

We found that chemical reactions of OCS and H atoms proceeded via quantum tunneling, mainly resulting in the dissociation of the C-S bond: OCS + H → OCSH, OCSH + H → H_2S + CO. Further hydrogenation of the products leads to the formation of formaldehyde and methanol and the desorption of H_2S by chemical desorption. Another product of potential importance in astrochemistry would be thioformic acid (HCOSH), which was formed by successive H addition to OCS[2], has been recently detected toward the quiescent cloud G+0.693–0.027[3].

Similar to the case of OCS, the reaction of CH_3SH with H atoms was found to have multiple channels: $CH_3SH + H \rightarrow CH_3 + H_2S$, $CH_3S + H_2$, or $CH_2SH + H_2$. The major channel was the dissociation of C-S bond in CH_3SH with the activation barrier of 0.05 eV on amorphous solid water, eventually resulting in the formation of methane (CH_4) by further hydrogenation to CH_3[4]. The hydrogen abstraction channels lead to the formation of CH_3S and CH_2SH radicals, and further hydrogenation to these radicals would result in the formation of CH_3SH again. Chemical desorption of CH_3SH was not positively identified via these processes, implying the presence of other processes for the desorption of CH_3SH from interstellar grains at low temperatures.

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P-04

Evolution of Crystalline Misorientations in Polycrystalline Samples of Pure Ice

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There are few studies where the evolution of grain orientations and crystal misorientations of neighboring grains in a polycrystalline ice sample during grain growth are analyzed. In this work, crystal orientations and misorientations were studied in two ice cylinders obtained from bidistilled water using the techniques of plastic replicas and chemical etching pits. The cylinders were grown, one through fast freezing and the other through slow freezing. It was observed that the initial crystal orientations of the grains varied from one cylinder to the other, but this did not result in significant differences in the final crystal misorientations between neighboring grains. Such crystal misorientations could be special because they are related to a coincidence sites lattice (CSL), which could be associated with low-energy grain boundaries. Therefore, the decrease in grain boundary energy during grain growth could be influenced by these special crystal misorientations.

P-05

In-Situ Observation of Pit on Ice Crystal Surfaces by Confocal Optical Microscopy

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Ice is involved in various phenomena occurring in the atmosphere, for example in the electrification of clouds, precipitation, and also as an agent on which numerous chemical reactions take place. All these phenomena are related to climate and environment. These things show why the study of the ice surface is a topic of great interest. [1-3]

A study of a pit on the surface of a previously polished single-crystal ice sample is presented. The evolution took place for three hours in the presence of activated silica gel, at a temperature of -5 ºC. Three-dimensional micrographs were taken every 15 minutes with an Olympus OLS4000 LEXT confocal microscope. The analysis of the micrographs made it possible to study the evolution of the well. Expressions obtained using the Mullins [4] and Srinivasan-Trivedi [5] models were used to describe the evolution of the observed profiles.

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P-06

Graph neural networks classify molecular geometry and deign novel order parameters of ice and water

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Conventionally, various order parameters are used to classify different structures of liquid and crystal. Conventional methods still require manual operation, such as exploring and calculating the order parameters. On the other hand, deep learning models are useful because they can automatically learn and classify structural features. However, it was difficult for the conventional deep learning model to make the learned features explainable because the classification accuracy is not very high.

In this work, we apply a types of graph neural network model, tensor embedded atom network (TeaNet)[1], to classify structures of ice 1h, ice 1c, and water. TeaNet achieved a highly accurate classification by an extremely small molecular structure, i.e. when the number of input molecules is 9, the accuracy is 99.8% (See Table 1). This is an advantage of our method over the conventional order parameters methods which require a large molecular structure. Furthermore, we verified that TeaNet can build novel order parameters without manual operation. Because TeaNet can recognize extremely small local structures with high accuracy, all structures can be mapped to a low-dimensional parameter space that can explain structural features (see Figure 1). TeaNet offers an alternative to conventional order parameters because of its novelty.

Table 1 Accuracy of classification by TeaNet.

Structure	Atom type	The number of molecule 3	 5	 7	 9
		Accurecy (Error)			
Ih vs liquid	O	0.693(0.0029)	0.920(0.0051)	0.994(0.0007)	**0.999**(0.0005)
	O+H	0.908(0.0026)	0.992(0.0012)	**0.999**(0.0004)	**0.999**(0.0002)
Ih vs Ic	O	0.488(0.0015)	0.489(0.0031)	0.789(0.0027)	0.924(0.0037)
	O+H	0.751(0.0048)	0.997(0.0007)	0.999(0.0004)	**1.000**(0.0002)
Ic vs liquid	O	0.684(0.0024)	0.920(0.0032)	0.997(0.0007)	0.999(0.0002)
	O+H	0.954(0.0011)	0.997(0.0003)	0.999(0.0010)	**1.000**(0.0002)
All	O	0.464(0.0048)	0.624(0.0003)	0.850(0.0038)	0.950(0.0046)
	O+H	0.765(0.0049)	0.992(0.0006)	0.997(0.0022)	**0.998**(0.0019)

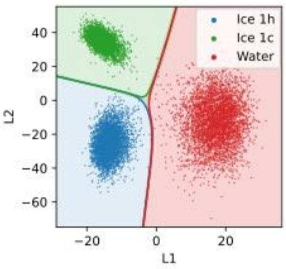

Figure 1 Novel parameters obtained by our method.

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P-07

A Molecular Dynamics Study of Low-Angle Tilt Grain Boundary Energies in Ice Bicrystals

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In this work, molecular dynamics was used to calculate the absolute grain boundary energies of ice bicrystals with low-angle misorientation. Starting with the crystalline structure of wurtzite, where oxygen atoms are located in their lattice sites, hydrogen atoms were then added using the Matsumoto Mazakasu algorithm [1]. Two series of symmetric tilt ice bicrystals were constructed with $\langle 10\bar{1}0\rangle/\Psi$ and $\langle 11\bar{2}0\rangle/\Psi$ low-angle misorientations. The selected misorientation angles were less than 20°, ensuring that the bicrystal structures had the lowest possible Σ value.

Grain boundaries were formed as an array of edge dislocations [2], considering the glide set of slip planes [3] to achieve the initial configuration with the lowest energy. The simulations were performed using the LAMMPS code, and the Tip4p/Ice potential [4] was employed. The energies were calculated at temperatures of 5 K and 250 K. The obtained values are consistent with the Read-Shockley model [5] and align with the experimental results obtained by Suzuki-Kuroiwa [6].

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P-08

Side-Branch Formation and its Direction during Growth of Snow Crystals

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Dendritic snow crystals are the most well-known crystals with regular and complex shapes. Its pattern formation has been thought to be determined by mass diffusion and surface kinetics. Recently, we used a Michelson interferometric system to measure the three-dimensional morphology of natural snowfall crystals [1] and artificial snow crystals in a diffusive chamber [2]. The morphology of these crystals was found to be a combination of a single flat basal plane and curved three-dimensional face with rib (ridge form). In addition, the water vapor supply side was found to be a flat basal plane [2].

Based on the observation by interferometric system, side-branches are formed by both morphological instability on prism plane and formation of macro step on basal plane [3]. On the other hand, on the opposite side of the basal plane of snow crystals, there are main and side ribs [4], as shown in Figure 1. The growth direction of the main ribs follows the crystallographic a-axis, while that of side ribs change to the crystallographic a-axis after the side-branch formation. This change in the growth direction of the side ribs will be discussed based on both the 3D structure and the surface diffusing water molecules.

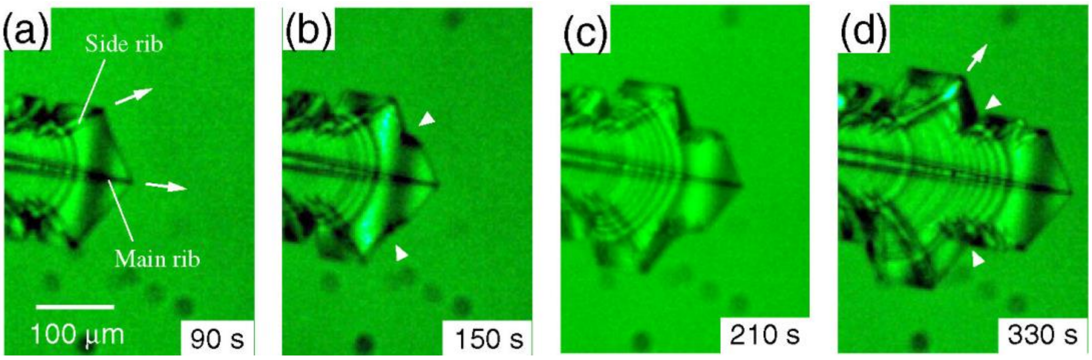

Figure 1. Time sequence of growing snow crystal with a flat basal plane (interference fringes) and a curved 3D basal face with ribs (silhouette).

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P-09

Grain Growth with Mobile Bubbles in Ice: Experiments and Numerical Simulation.

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Hailstones in the clouds grow under different environmental conditions (temperature, humidity, wind, etc.), and these conditions affect the size and texture of the ice grains. The stratified structures within a hailstone provide information about its growth stages. Given the countless trajectories that can exist and the varying environmental conditions, it is expected that many disruptions in the characteristics of hailstones occur within the same storm. Therefore, extracting information about a storm based on the characteristics of hailstones poses a real challenge.

The grains, in each stratified region of hail, grow containing a large number of bubbles inside and on the grain boundaries. As hail forms, its grains continue to grow over the time that the hail remains in the thunderstorm cloud, and after it has fallen to the ground. Grain growth is a thermally activated process but also depends on atmospheric contaminants that are collected within the cloud and the bubbles on the grain boundaries.

This study examines the evolution of grain size in a sample of bubbly ice using theoretical equations and a Monte Carlo-based growth model. The computational and theoretical results are applied to laboratory-grown bubbly ice samples, enabling the description of grain boundary mobility in ice and its interaction with existing bubbles. The results demonstrate that the bubbles move with the grain boundaries but produce a slowing effect on them. This leads to the conclusion that bubbles would help preserve the crystallographic and morphological information of hail when exposed to temperatures near the melting point.

P-10

Impact strength of porous icy bodies in high-velocity oblique collision: Implication for catastrophic disruption of Kuiper belt objects in outer solar system

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It is important to examine the “impact strength” of porous ice in order to investigate the collisional evolution of Kuiper belt objects in the outer solar system. Some researchers have conducted impact experiments to examine the impact strength of ice as a function of porosity. Here, we focus on the effect of impact angle since the solar system bodies collide at different impact angles. In this study, oblique impact experiments of ice balls were conducted to examine the effect of impact angle on impact strength.

Impact experiments were conducted using a two-stage light gas gun at Kobe University. We prepared two types of spherical targets with diameters of 60 to 80 mm. One is non-porous water ice and the other is porous ice (snow) with 50% porosity. Polycarbonate or glass projectiles with a diameter of 2 or 4.7 mm were used. Impact velocities ranged from 0.7 to 5.1 km/s. The impact angle θ was varied from 15º to 90º (head-on collision). The collisional phenomenon was observed with a high-speed camera.

The specific energy Q, which is the kinetic energy of the projectile divided by the target mass, is used to determine the impact strength. Impact strength, Q^*, is defined as Q when the largest fragment mass is half of the original target mass. Fig. 1 shows the relationship between the largest fragment mass normalized by the original target mass m_l/M_t and the Q. The m_l/M_t of snow targets was larger than that of ice targets. On the other hand, the m_l/M_t for impact angles less than 30º were larger than those greater than 40º for both targets. We introduced the specific energy $Q_{\mathrm{eff}} = Q\sin^2\theta$, including the impact angle and reanalyzed the results. This resulted in one empirical equation describing the relationship between the m_l/M_t and the Q_{eff} for each target, yielding modified impact strengths $Q_{\mathrm{eff}}{}^*$ of 16 and 492 J/kg for ice and snow targets, respectively.

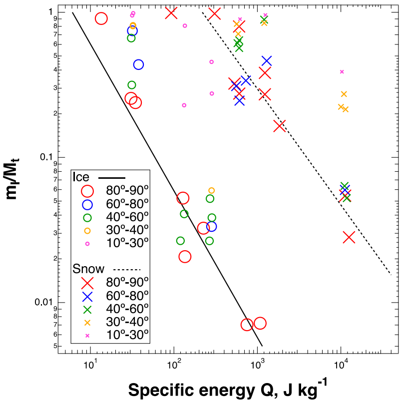

Fig. 1: m_l/M_t vs. Q at various impact angles.

P-11

Experimental study on collisional disruption of differentiated icy planetesimals

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Icy bodies such as icy satellites and comets in the solar system are thought to have grown through collisions and re-accumulation of icy planetesimals. In addition, when icy satellites exceed 500 km in diameter, the interior have a layered structure depending on the density, or is completely differentiated into a core and mantle structure. Therefore, it's important to understand the collisional processes considering the internal structure of icy planetesimals in order to clarify the evolution of icy bodies. So far, many laboratory impact experiments have been conducted to investigate the collisional processes of solar system icy bodies, but most of them used targets with homogeneous structures such as only ice and only snow. In this study, we conducted high-velocity impact experiments using a layered structure target with a snow mantle around an ice core and obtained the cumulative number distribution of impact fragments and impact strength to investigate the degree of collisional disruption.

Impact experiments were conducted using a two-stage light gas gun installed at Kobe University. The projectile was a polycarbonate sphere with a diameter of 4.7 mm, and the impact velocities were 1 km/s and 2 km/s. The spherical target with a diameter of 60 mm had a layered structure with a snow mantle of 50% porosity around a non-porous ice core with a diameter of 30 mm. The collisional phenomena were observed by two high-speed cameras from different directions.

Cumulative number distribution of impact fragments showed that the largest fragment of the layered target originates from the mantle, and the degree of core fragmentation is smaller than that of mantle, indicating that the mantle fragmentation dominates the size distribution of impact fragments. Comparing the impact strength of a homogeneous snow target in this study with that of snowballs (50% porosity) (Nakamura, 2020)[1], the impact strength in this study was smaller than that obtained by Nakamura. This difference was expected to be due to the difference in impact velocity. For the homogeneous snow target, cracks grew radially from the impact point. On the other hand, in the layered target, fine cracks were observed in the mantle, and mantle was pushed out faster from the core-mantle boundary in the direction perpendicular to the impact axis. This might be caused by the pressure gradient at the boundary between the ice core and the snow mantle during the collision.

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P-12

Preliminary Results of Dielectric Profile Measurements of Ice Cores From the Flank of the Dalk Glacier, Antarctica

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The electrical properties of ice cores are one of the most significant physical indicators for ice core studies, including electrical conductivity and permittivity. Results can be applied to dating of ice cores, study on ice sheet accumulation rate and impurity concentration (analysis of volcanic events). In the analysis of the electrical properties of ice cores, Dielectric Profiling (DEP) uses electrodes with low voltage and high frequency alternating current to measure the conductivity of solid ice. DEP has the advantages of fast measurement speed and having little damage to ice core samples. The use of electrical conductivity data for analysis of volcanic events can also synchronize dating between multiple deep ice cores, such as EGRIP, NEEM, and NGRIP in Greenland [1].

Three ice cores were analyzed by DEP in a low-temperature laboratory at -15 ℃, which were drilled at the front lateral margin of Dalk Glacier, East Antarctica. The results show that the electrical conductivity and permittivity of the ice cores show multi-decadal variations with the depth. This study provides a reference for future studies on the 198m Ice core through the bottom drilled in the same area.

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P-13

Cellulose Nanofibrils Tune the Mechanical, Optical, and Thermal Properties of Ice

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Ice is an abundant natural resource in cold regions, and ice often naturally contains particulates and organic fibers that can affect the material properties. The presence of impurities and second phase materials in ice during freezing can drastically change the ice microstructure, and therefore modify the macroscopic properties of the resulting composite material. Cellulose nanofibrils (CNFs) are natural fiber bundles that have shown promise for reinforcing ice for construction use [1, 2]. We have used several different techniques to examine the changes to the thermal, mechanical, and optical properties of the ice when reinforced with different concentrations of CNFs.

The addition of cellulose nanofibers to the ice results in smaller and less uniform grains as the fibers influence ice grain growth during freezing. Our microscopy revealed that entrapped CNFs in the ice matrix occur both within and between the grains of ice and are not confined to the grain boundaries. This, along with the reduced grain size, results in an increase in the flexural and compressive strength of the ice reinforced with cellulose. We also observed a change in the heat transfer in the cellulose reinforced ice due to lowered thermal conductivity, reduced radiative absorption from increased reflectivity, and reduced convective heat transport from an insulating layer of CNFs that forms on the surface of the ice during melting. The changes in the mechanical, thermal, and optical properties of the cellulose reinforced ice make CNFs an ideal second phase material to modify ice for use in ice structures in cold regions.

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P-14

High pressure Plastic Phases of water and water-ammonia mixtures

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The ‘ice giants’ Uranus and Neptune, as well as some of their moons and many Neptune-like exoplanets, are mainly composed of mixtures of three molecular ices: water, ammonia and methane. All these molecular crystals show plastic phases. For methane [1] and ammonia [2] these phases are already known experimentally, while for water and ammonia hydrates only numerical simulations exist [3,4]. From the dynamical point of view the plastic phase is an intermediate phase between a liquid and a crystal: molecules are held tightly in an ordered structure, but can rotate as in a liquid state. We will present the characterization of the plastic phases of water [5] and of ammonia monohydrate [6] by high pressure quasi elastic neutron scattering (HP-QENS) experiments performed at ILL, Grenoble. Measurements up to 8 GPa show that ammonia monohydrate’s phase VII is a rotor phase [6], similarly to methane and ammonia. For water instead the plastic behavior is different, the rotation occurs by orientational jumps trough multisite positions in the lattice, resulting in a more complex $S(Q,\omega)$ profile which is here modelled through MD simulations [5].

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P-15

Ultra-High Vacuum Cryogenic Transmission Electron Microscopy of Ices Indicates the Possible formation of Hydrogen-Ordered Ices

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Transmission electron microscopy (TEM) is suitable for observing a sample and its crystalline structure in nanoscale simultaneously. However, with conventional TEMs, formation of ice under controlled conditions is difficult because the partial pressure of water vapor inside the column of TEM is not sufficiently low to avoid the continuous deposition of water on the cryogenic samples. To solve this problem, an ultra-high vacuum cryogenic transmission electron microscope was developed [1,2], which enables not only observation of samples at ultra-high vacuum ($\sim 1\times10^{-6}$ Pa) and low temperatures (6–170 K) but also ice formation with controlled partial pressure of water vapor using gas inlet tubes. In this study, using this apparatus, hydrogen-disordered ices I were deposited on an amorphous silicon nitride thin film as a substrate and their structural changes during annealing processes were investigated.

Some electron diffraction spots were observed in the electron diffraction patterns from observed ices, which are not commonly observed in ice Ih and Ic. To determine the origin of these spots, we calculated the d-spacings and relative intensities of ice phases such as hydrogen-ordered ices I [3,4] and stacking disordered ices I [5]. We plan to discuss the possibility of the formation of hydrogen-ordered ices I by simple annealing of disordered phases of ices I.

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P-16

Study of Concentration-Cooling Rate Map of Ice in Aqueous Polymer Solutions by X-ray Diffraction Measurements

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Introduction

It is well known that there are various ice crystal structures depending on temperature and pressure. Three types of ice exist under atmospheric pressure [1]. The type of ice in aqueous solutions are affected by the presence of solute. In this study, we create the Concentration-Cooling rate Map (CCM) for aqueous polymer solutions, which represents the variation of ice depending on polymer concentration and cooling rate, using X-ray diffraction measurements. We discuss the CCM in terms of kinetics of water such as local viscoelasticity during ice formation process.

Experiment

The polymer used in this study was poly (vinyl pyrrolidone) (PVP) with weight-average molecular weight of 10000 g/mol purchased from Sigma-Aldrich. Deionized water with a resistivity of 18.2 MΩ cm purified by Simplicity UV (Merck Millipore) was added to PVP to prepare aqueous solutions of PVP with PVP concentrations up to 55 wt. %. The temperature of the aqueous solutions of PVP were cooled from 10 ℃ to -70 ℃ at cooling rates ranging from 1 to 100 ℃/min. X-ray diffraction measurements were performed at -70 ℃ using XtaLAB PRO P200 (Rigaku Corporation).

Result and Discussion

The CCM of ice in aqueous PVP solutions was created. The X-ray diffraction peak patterns of ice Ih was observed at lower PVP concentrations and slower cooling rates. As the PVP concentration and cooling rate increased, the X-ray diffraction peak patterns of ice Isd was observed, further increasing, non-crystalline system without peaks due to ice were observed.

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P-17

Pressure dependence of dynamics in high-density amorphous ice

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Water is the most normal liquid to us due to its daily presence in our life. However, it has various anomalous properties as a liquid from scientific point of view. Its properties diverge from normal liquid's behavior at supercooled temperatures. Interestingly, according to theoretical studies [1] water can exist as two different liquid states. Those liquid states are named as high- and low-density liquid (HDL and LDL). The two-liquid-states model became particularly interesting due to experimental reports on two different amorphous solid states of water: high- and low-density amorphous ices (HDA and LDA) which are suggested to be their corresponding glassy states according to the model. While the glass-liquid transition of LDA to LDL can be studied at ambient pressure (T_{g1} = 136 K), both HDA and HDL are stable at elevated pressures. In most of the reported studies, HDA, prepared by compression in a mechanical press, is quench-recovered by adding liquid nitrogen and studied at ambient pressure [2].

The poster provides an overview of recent experiments on HDA's dynamics at ambient and elevated pressures studied by X-ray Photon Correlation Spectroscopy (XPCS) [3]. XPCS is a powerful technique to determine viscous dynamics in glasses using coherent X-rays. Thereby, scattering intensity fluctuations obtained from sample heterogeneity are correlated over time. Measuring in small-angle geometry, we determine a collective motion and the related relaxation time of the system. Our high-pressure cryogenic setup allows us to investigate the glass transition in HDA at elevated pressure.

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P-18

Structure and Dynamics of Vapor-Deposited Amorphous Ice

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Water vapor-deposited at low temperatures (below 140 K) forms an amorphous solid known as amorphous solid water (ASW) [1]. Although rare on Earth, this form of water is abundant in outer space [2]. Understanding the properties of vapor deposited solid water not only plays an important role in astrophysics, but its relationship with liquid water is an integral piece in the puzzle that is the phase diagram of supercooled water.

Deposition at liquid nitrogen temperature results in a microporous material [2]. Upon heating beyond 120 K, the cylindrical pores collapse into 2D lamellae [3]. This structural change was characterized by small-angle neutron diffraction as a process originating from translational diffusive motion [4].

In a recent experiment, we studied the nanoscale dynamics of amorphous solid water with X-ray photon correlation spectroscopy (XPCS). A two-detector setup allowed us to measure dynamics and pore surface area (small-angle scattering), while simultaneously monitoring the molecular structure (wide-angle scattering). With two species of sample – bulk powder prepared *ex situ* and thin film deposited *in situ* – we did experiments both in transmission and in grazing incidence geometry. By stepwise heating up to complete pore collapse, quenching, and reheating, we investigated the influence the presence of pores and their collapse has on the diffusive dynamics of amorphous solid water.

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P-19

Temperature and Pressure effects on the transformation of Ices

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In the presentation, we report recent results on the investigation of structural changes of vapour-deposited amorphous and pressure-amorphized ices using time-dependent synchrotron x-ray and neutron diffraction, respectively. The sequence of transformations from rapidly condensed water to crystalline ice is found to depend on the presence of co-deposited foreign molecules. The known sequence from amorphous – stacking disordered – crystalline is reproduced for the pure system. It is found that the First-Shape-Diffraction Peak (FSDP) of amorphous ice merges to the (001) Bragg reflection in crystalline ice, indicating nascent short-range hexagonal ordering is already present in amorphous ice. In contrast, at the high concentration of nitrogen, successive crystal-crystal transformations of solid nitrogen, mixed with an amorphous halo pattern were observed at low temperatures. Surprisingly, crystalline ice features occur immediately after the melting of the nitrogen. In contrast, at lower nitrogen concentrations, a small amount of crystalline nitrogen mixed with amorphous ice was observed with the FSDP at ~ 1.9 $Å^{-1}$, very close to that of high-density amorphous (HDA) ice. The position of the FDSP decreases with increasing temperature and approaches that of low-density amorphous ice at ~1.7 $Å^{-1}$ before transforming to stacking-disordered ice at 140 K.

Neutron diffraction was used to characterize the pressure-induced amorphization of crystalline ice. Contrary to an earlier report, no crystal-crystal transformations were observed at 100K with prolonged annealing. Instead, HDA always coexists with dense forms of ice. Remarkably, only pure amorphous ice was identified below 90 K and in a very narrow temperature region around ~140K. At slightly higher temperatures, the expected thermodynamic crystal-crystal transformations were observed. The results indicate there are two competing mechanisms when crystalline ice is compressed.

P-20

Effects of anti-freeze glycoproteins on long-term storage of cryopreserved trehalose-transporter expressing cells and on ice recrystallization

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We have studied cryopreserving the cells expressing a transporter (TRET1) that can transport trehalose into cells to investigate the function of trehalose as a cryoprotectant. It was found that the viability was highest when both intra- and extracellular trehalose concentration are about 0.5M [1]. When these cells were stored at -80°C, the viability was maintained high for one year, but it decreased after that [2]. One of the reasons for this viability reduction is thought to be ice recrystallization. So, we examined the effects of anti-freeze glycoprotein (AFGP), as a inhibitor of ice recrystallizations, on the viabilities and ice crystal sizes during one-year storage period.

The TRET1-expressing CHO-K1 cells were dispersed at 10^5-10^6 mL^{-1} in a freezing solution, in which both 0.4M trehalose and 0 ~ 0.5 g/L AFGP were added. 1 mL of cell-dispersed solution was frozen and stored at -80, -60 and -40°C. The frozen samples were taken out at fixed intervals, thawed quickly, and measured the viabilities by a flow cytometer. Ice crystals prepared by quenching the freezing solutions between coverslips in liquid nitrogen were also stored in the same temperature environments, and its size was measured by a microscope. We found that the viability decreased during about 2 months and became almost stable after that. Since the ice recrystallization occurred significantly at the same time, we consider that the decreasing in viability would be caused by the ice recrystallization. The addition of AFGP reduced the ice recrystallization rate, so the viabilities might be improved indirectly.

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P-21

Lichen Species Produce Highly Active and Stable Ice Nucleators

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Forty years ago, lichens were identified as extraordinary biological ice nucleators (INs) that enable ice formation at temperatures close to 0°C. By employing INs, lichens thrive in freezing environments that surpass the physiological limits of other vegetation, thus making them the majority of vegetative biomass in northern ecosystems. Aerosolized lichen INs might further impact cloud glaciation and have the potential to alter atmospheric processes in a warming Arctic. Despite the ecological importance and formidable ice nucleation activities, the abundance, diversity, sources, and role of ice nucleation in lichens remain poorly understood. Here, we investigate the ice nucleation capabilities of lichens collected from ecosystems across Alaska. We find ice-nucleating activity in lichen to be widespread, particularly in the coastal rainforest of Southeast Alaska. Across 29 investigated lichens, all species show ice nucleation temperatures above -15°C and ~30% initiate freezing above -6°C. Concentration series of lichen ice nucleation assays in combination with statistical analysis reveal that the lichens contain two subpopulations of INs, similar to previous observations in bacteria. However, unlike the bacterial INs, the lichen INs appear as independent subpopulations resistant to freeze-thaw cycles and temperature treatment. The ubiquity and stability of the lichen INs suggest that they can impact local atmospheric processes and that ice nucleation activity is an essential trait for their survival in cold environments. Additional research is needed to characterize the lichen INs to evaluate the nature of the macromolecules responsible for ice nucleation and the abundance of lichen INs in environmental samples on a global scale.

P-22

The Role of Antifreeze Proteins in Cellular Membrane Stabilization

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Cold-adapted organisms face the continuous challenge of unwanted ice crystal growth and cellular damage when exposed to subfreezing temperatures. To overcome these challenges, organisms thriving in icy environments have evolved antifreeze proteins (AFPs) and antifreeze glycoproteins (AFGPs) that can prevent macroscopic ice crystal growth. Additionally, AF(G)Ps are thought to prevent leakage of intracellular metabolites by stabilizing cellular membranes through the phase transition. Here, I present the effects of different AF(G)Ps on model lipid membrane systems when exposed to colder temperatures. By understanding the underlying mechanisms of AF(G)Ps and lipid membrane interactions, these proteins might be employed in future biomedical applications to better preserve cells, tissues, and organs.

P-23

Studying the Decisive Factors for Maximum Freezing Efficiency of Bacterial Ice Nucleators

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Bacterial ice nucleators (INs) initiate ice crystal growth with exceptional proficiency reaching freezing temperatures close to 0°C by employing specialized ice-nucleating proteins (INPs) anchored to the outer bacterial cell membrane. While the exact working mechanism remains still under debate, the high freezing efficiency is linked to the formation of functional INP aggregates providing an accumulated ice-binding site [1]. Further, freezing assays reveal a broad range of nucleation temperatures with distinct areas of enhanced IN activity. This suggests the presence of variously sized aggregates, the exact dimensions of which remain undetermined. Here, we present the decisive factors that control the formation and stability of functionally aligned INP aggregates by combining high statistical droplet freezing assays with advanced physicochemical approaches. We find the bacterial cell membrane state and environmental conditions crucial for enabling precise assembly and thus, maximum freezing efficiency [2]. By shedding light on the complex formation of INP aggregates, we achieved a more proper picture of the mechanism behind bacterial ice nucleation.

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P-24

Sources of perchlorate in Antarctic Snow

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Perchlorate (ClO_4^-), a persistent inorganic compound, is harmful to human health [1]. Environmental ClO_4^- has both anthropogenic and natural sources. Anthropogenic sources mainly derive from the extensive use of man-made perchlorate salts as an oxidant in rocket propellants, pyrotechnics, and munitions [2]. Natural ClO_4^- is widespread in the environment [3], however, knowledge gaps remain in its levels, potential sources, and production mechanism. Antarctic snow provides one of the best records to investigate natural ClO_4^-. Results show that ClO_4^- in Antarctic snow is dominated by atmospheric production, with nearly no human inputs [4]. Perchlorate concentration, in the range of a few to a few hundred ng kg^{-1}, exhibits an obvious increasing trend since 1970s, which may be the result of the elevated stratospheric chlorine levels by anthropogenic chlorine emissions [5]. Perchlorate in summer snow in coastal Antarctica may predominantly originate from tropospheric chemistry; while a significant amount of ClO_4^- in summer snow in interior East Antarctica may be of stratospheric origin [6]. Seasonal variation of ClO_4^- shows that the timing of ClO_4^- minimum is simultaneous with total column ozone minimum [5], indicating that significant atmospheric ClO_4^- formation in the Antarctic stratosphere may begin to occur when stratospheric ozone depletion appears [4].

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P-25

Sulfate concentration and electrical conductivity of firn cores at Vostok (central Antarctica) as proxy of volcanic activity over the past 2,200 years

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The products of volcanic eruptions found in the snow, firn and ice deposits of the polar ice sheets are precious sources of information on the volcanic forcing of the climate system in the recent or remote past. Also, the layers containing the traces of well-known eruptions serve as absolute age markers that help to construct the depth-age scale for the snow-firn thickness [1].

In this study we present new records of the sulfate concentrations and electrical conductivity (ECM) from three shallow (up to 70 m depth) firn cores – VK16, VK18, VK19 – drilled in the vicinity of Vostok station (central East Antarctica). In the non-sea-salt sulfate and ECM profiles we were able to identify 68 peaks that can be interpreted as traces of volcanic events: 22 peaks can be unambiguously attributed to well-known volcanic eruptions, which are used as foundation of our age model; 37 events have their counterparts in other Antarctic cores, but cannot be associated with well-dated eruptions; 9 peaks do not have analogues in the other cores.

According to the newly constructed depth-age function, the deepest studied firn layers (70.20 m) are dated by 192 BCE.

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P-26

Toward New Impregnation-Refreeze Products for Tomography of Snow Samples?

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Characterizing snow by microtomography (μCT) often requires adding an impregnation liquid that fills into the pores and can easily freeze when lowering the sample's temperature. This impregnation-refreeze process is intended to (1) preserve the snow samples from metamorphism and (2) strengthen the snow structure before machining and imaging the sample. To date, the most used chemical is "1-chloronaphthalene", which has shown very good results, especially in terms of machining and X-ray contrast [1]. However, it remains a product that requires some precautions due to its hazard classification. Several authors have proposed two diethyl phthalate (DEP) based approaches as alternatives to chloronaphthalene: 1) a replica vacuum-based approach [2], and 2) a technique using DEP doped with I2 and BaTiO3 nanoparticles, to increase the DEP to ice contrast [3]. Yet, each of these approaches requires a relatively complex preparation and raises some questions on its practical usage, especially for high resolution imaging.

In this work, several impregnation-refreeze experiments on depth hoar have been carried out for more than 20 chemical products of interest. After refreezing, the samples have been characterized by μCT and subsequently evaluated based on their image quality.

The first results obtained, with sometimes notable variations in X-ray absorption, demonstrate different important aspects of snow impregnation and refreezing depending on the products used. These results will allow further progress in the ongoing research for the most suitable products.

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P-27

Guest Gas-Induced Structural Transformation of Tetra-n-butylammonium Chloride Semi-Clathrates

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Gas hydrates are crystalline inclusion compounds in which guest molecules are encapsulated within host water frameworks. Semi-clathrates share many physical and chemical properties with gas hydrates, but in semi-clathrates, guest anions can participate in forming the host water frameworks. Quaternary ammonium salts such as tetra-n-butylammonium chloride (TBAC) form semi-clathrates with water. Pure TBAC semi-clathrate was reported to have a tetragonal ($P4_2/m$) structure [1].

In this study, the possible structural transformation of TBAC semi-clathrates in the presence of Xe or Kr was experimentally investigated with a primary focus on semi-clathrate phase equilibria and spectroscopic and crystallographic measurements. The slopes of the three-phase (clathrate (H) – liquid (L) – vapor (V)) equilibrium curves for the TBAC + guest gas + water systems altered at one or two points as the pressure and temperature increased. Powder X-ray diffraction (PXRD) patterns clearly demonstrated that when Xe or Kr molecules were captured in TBAC semi-clathrates, their structure changed from tetragonal ($P4_2/m$) to orthorhombic ($Pmma$) structure. *In-situ* Raman spectroscopy was additionally used for TBAC + Xe semi-clathrate, whereas high-pressure micro-differential scanning calorimetry (HP μ-DSC) was utilized for TBAC + Kr semi-clathrate to examine the existence of multiple structures and resulting structural transformation of the semi-clathrates. The experimental results indicated that inclusion of guest gases of Xr or Kr in the small cages of semi-clathrates induced structural transformation especially at high pressures.

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P-28

Effect of functional group in dicarboxylate anions on the latent heat storage properties of semiclathrate hydrates

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Semiclathrate hydrates (SCHs) have been expected to be one of the phase change materials suitable for cold energy storage. One of the significant characteristics of SCHs is the equilibrium temperature can be changed to an expedient temperature for a target material by the cation, the anion, or both in the guest quaternary onium salts[1]. In the present study, equilibrium temperature, dissociation enthalpy, and crystal structure of tetra-*n*-butylphosphonium dicarboxylate (TBP-DC) SCHs[2], where the dicarboxylate anions were Oxalate (-Oxa), Malonate (-Mal), Succinate (-Suc) and Glutarate (-Glu), were investigated. In addition, to investigate the effects of hydroxycarboxylate (-HC) on the equilibrium temperature and the dissociation enthalpy, TBP-HDC SCHs with Malate (-Mala, addition of a hydroxy group to -Suc) and Tartrate (-Tar, addition of two hydroxy groups to -Suc) were investigated. Changing the methylene chain length and introducing the hydroxy groups affect the equilibrium temperature and the dissociation enthalpy of SCH largely. The methylene chain length and hydroxy groups could be a way to design the SCHs with desired equilibrium temperatures.

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P-29

Investigating the Possibility of C_3F_8 as a Gaseous sH Hydrate Former

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sH hydrates have larger gas storage capacity potential and require milder hydrate-forming pressures compared to sI and sII hydrates, making them an attractive option for hydrate-based gas storage and transportation. Traditionally, large-sized organic liquids, which occupy large ($5^{12}6^8$) cages, have been used to form sH hydrates [1]. However, in this study, C_3F_8 was proposed as a new gaseous sH hydrate former. C_3F_8 is a thermodynamically stable and non-flammable gas, and thus, it has been useful in various industrial fields such as medical processing and semiconductor manufacturing [2]. The phase equilibrium curve of the C_3F_8 + CH_4 hydrate was shifted to the lower pressure region as compared to pure CH_4 hydrate, implying the participation of C_3F_8 in the hydrate cages. The enclathration of C_3F_8 into sH hydrate cages in the presence of CH_4 was clearly observed by spectroscopic and crystallographic methods including Raman spectroscopy, NMR, and PXRD. The findings of this study clearly demonstrated the potential of C_3F_8 as a unique gaseous sH hydrate former.

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P-30

Effect of Gas and Water Flow Velocities on Flow Patterns and Gas Uptake of Hydrate Slurries in a Scaled-up Vertical Plug Flow Reactor

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Gas hydrates that gas molecules are selectively captured by thermodynamic properties enable us to utilize hydrates as a gas separation material. There is still little information on mass transfer for hydrate-based gas separation. We have conducted gas uptake experiments in a vertical plug flow reactor with a static mixer [1]. However, the setting ranges of gas and water velocities were limited because of the problems of gas backflow and pipe blockage. This research aims to clarify the effects of gas and liquid flow velocities on the flow patterns and gas uptake performance of hydrate-based gas separation when the reactor is scaled up.

The experimental apparatus was scaled up to twice the diameter of the previous apparatus [1]. A gas mixture of HFC-134a and nitrogen was used as a model gas for greenhouse gases. Gas hydrate was formed by countercurrent contact between the gas mixture and water in this apparatus. The flow patterns were visually observed. The liquid-side volumetric mass transfer coefficient was calculated to evaluate the gas absorption performance.

Bubbles often rose along the twists of the element in the apparatus, and many fine bubbles were observed. This result suggests that fine bubbles were generated due to shear forces between the elements and bubbles or between hydrates and bubbles. The mean bubble diameter increased with increasing gas and liquid flow velocities, and the liquid-side volumetric mass transfer coefficient during hydrate formation decreased.

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P-31

Raman spectroscopic investigation of clathrates formation including C_3F_8 with various help gases

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One of the perfluorocarbons, octafluoropropane (C_3F_8, or R-218) is widely used in several industrial fields, such as the semiconductor manufacturing and the medical applications since it is non-flammable and thermodynamically stable. However, it is also known to be one of the global warming gases (GWP ~ 7000). To sequestrate it from the emission source, the utilization of gas-hydrate formation is one of the expected processes. Since C_3F_8 is larger than propane (C_3H_8), it is known to form sH hydrate with methane (CH_4) as a help gas. In the present study, we investigated several small guests whether they are able to be a help gas for enclathrating C_3F_8 in the hydrate phase.

We used the micro-Raman spectroscopy system (SPEX Raman 750, Ar^+ laser of 514.5 nm at 30 mW, and 1800 mm^{-1} grating) and a high-pressure vessel equipped with a sapphire glass (Taiatsu Techno Co.). About 20 μL pure water was set in the vessel, and high purity C_3F_8 (Tomoe Shokai Co., Ltd.) mixing with another help gas at a set experimental composition were pressurized. The experimental pressure was selected more than their dissociation pressures of single-gas hydrates, and less than their saturated pressure at fixed experimental temperature, about 274 K. The tested small guests are hydrocarbon gases (CH_4, ethane (C_2H_6) and C_3H_8; Air Water Hokkaido Inc.), inert gas (xenon; Air Water Hokkaido Inc.) and carbon dioxide (CO_2; Sankemi Co, Ltd.), where CH_4, C_2H_6, CO_2 and xenon form sI structure as single-gas hydrates, and C_3H_8 forms sII hydrate. Raman spectra of enclathrated C_3F_8 were obtained on CH_4 and C_3F_8 mixed-gas hydrate. We find that C-C stretching mode of Raman spectra of C_3F_8 shifts approximately 2 cm^{-1} lower than that in vapor phase. Using this shift change, we determined the enclathration of C_3F_8 molecules in various help gases.

P-32

Evaluation of Mass Transfer during Clathrate Gas Hydrates Formation by Using Dimensionless Number

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Clathrate hydrates are nonstoichiometric crystalline compounds composed water and gas molecules under the temperature and pressure conditions depended on a gas species [1]. The gas separation technology by using this characteristic is actively studied. We focused on a mass transfer during gas hydrates formation. The study aims to organize the mass transfer property in gas hydrate formation by using dimensionless number Sherwood number (*Sh*), Schmidt number (*Sc*) and so on.

The HFC134a-N_2 gas mixtures were supplied into water in a flow-type tube device equipped a Kenics-type static mixer. After the gas were saturated with water, hydrates were formed at 278 K and 0.325 MPa. Outlet gas flow rates during a gas saturation and hydrate formation were recorded.

A mass transfer rate of HFC134a gas molecules during hydrate formation was calculated from the deference the inlet and outlet gas flow rate. Based on the equation of mass transfer by using dimensionless number in gas-liquid systems proposed by Fukuma et al. [2], we organized the mass transfer of HFC134a gas during hydrate formation by dimensionless number.

Experimental values of *Sh* were lower than calculation values of *Sh*. This result implies that the mass transfer between the gas and hydrate slurry during the hydrate formation was inhibited by the hydrate films on the bubble surface.

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P-33

Pressure-induced phase transformations and their pressure hystereses of nitrogen hydrate

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Nitrogen hydrate is known to form a cubic structure II (sII), and it successively transforms into a hexagonal structure H (sH) at 0.8 GPa, a tetragonal structure T (sT) at 1.3 GPa, and an orthorhombic structure O (sO) at 1.6 GPa by compression[1]. Moreover, the high pressure Raman study and microscopic observation indicated the possibility of the doubly occupied large cages ($5^{12}6^{4}$) by nitrogen molecules above 0.5 GPa in the sII phase[2]. Therefore, the purpose of this study is to clarify the double occupancy in the sII phase by detailed high pressure X-ray powder diffraction measurements for nitrogen hydrate.

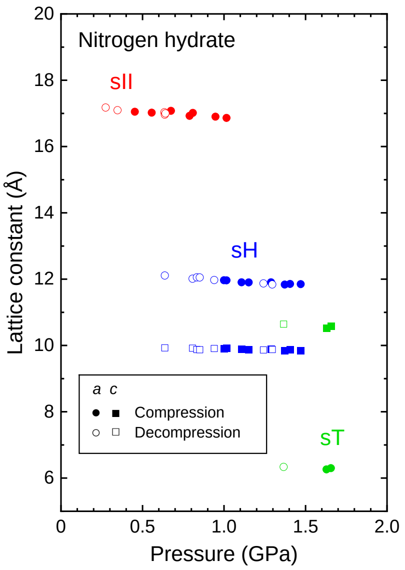

Fig. 1 The pressure dependence of the lattice constants of nitrogen hydrate.

Fig. 1 shows the pressure dependence of the lattice constants of nitrogen hydrate. A small jump of the lattice constant of sII was found at around 0.6 GPa. This jump suggests the volume expansion by the change of the occupancy in the $5^{12}6^{4}$ cage. In addition, we also found the pressure hystereses of 0.64-1.02 GPa (sII-sH) and 1.37-1.47 GPa (sH-sT). The large hysteresis between sII and sH possibly implies the instability of sII above 0.6 GPa.

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P-34

Supercooling suppression in the tetrahydrofuran clathrate hydrate formation

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With the demand for efficient and environmentally friendly transportation systems, latent heat storage technology draws attention. An example of applications is cold transportation of fresh foods and medical vaccines, in which a latent heat storage material is packed and kept cold to maintain freshness and effectiveness. Since it is not necessary to carry refrigeration equipment simultaneously, it achieves weight reduction and distribution cost reduction. For further efficiency enhancement, it is important to reduce the degree of supercooling. The large degree of supercooling is not preferable because extra cooling energy is required to crystallize cold storage materials.

Tetrahydrofuran (THF) clathrate hydrate is a cold storage material having a latent heat temperature of 277.45 K and a large amount (250 J/g) of latent heat. However, due to the large degree of supercooling, generally it does not crystallize unless cooled to 253 K. We have investigated how to suppress supercooling in the clathrate hydrate formation mainly by utilizing TEM and freeze-fracture replica method [1-3]. In this presentation, we will report the results on supercooling suppression in the THF hydrate formation by Raman spectroscopy as well as TEM and freeze-fracture replica method.

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P-35

Rheological Properties of SF_6 Gas Hydrate Slurry with Surfactant in Horizonal Circular Pipe

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Hydrate-based gas separation is attracting attention as a new gas and recovery method for greenhouse fluorinated gases. Gas hydrate slurries are said to be non-Newtonian fluids, but the practical application of hydrate slurries requires precise knowledge of their flow characteristics. This study aims to clarify the flow pattern and rheological properties of SF_6 gas hydrate slurry. Besides, the properties of SF_6 gas hydrate slurry with a surfactant as a dispersant were investigated.

The loop tube-type flow apparatus was used [1]. The pressure drop was measured under the conditions of a solid fraction of 0~13 vol% and the flow rate of 0.1 ~ 2.0 L/min. Sodium dodecyl sulfate (SDS) was used as a surfactant. The flow pattern of the slurries was visually observed. In the pseudo-homogeneous flow, the rheological properties were assessed using the apparent viscosity calculated with the shear stress and the shear rate at the wall. In a low solid fraction, the apparent viscosity was almost constant regardless of the shear stress, which shows that the slurry was a Newtonian fluid. In high solid fraction, the apparent viscosity decreased with increasing shear rate, which showed the tendency of pseudoplasticity. These results indicate that the interaction between hydrate particles affects the fluid properties in the high solid fraction. When SDS was added in the slurry, the apparent viscosity became lower than that without SDS. This result indicates that SDS molecules inhibit particle agglomeration and consequently the interparticle friction decreases. It was found that SDS has an agglomeration inhibit effect.

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P-36

DFT Calculations of Raman Spectra and NMR Shielding Constants for Large Clusters of Methane Hydrate

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Ramana and NMR spectra measurements for gas hydrates are fundamental experiments to study their specific features. But DFT calculations of these spectra are usually performed for the small and large cages of gas hydrates. To elucidate the effect from neighboring cages, DFT calculations for large clusters consisted of a small or large cage and surrounding small and large cages were performed using Gaussian16[1] on the super computer system of Hokkaido University. NMR shielding constants of C atoms of methane molecules were calculated at ωB97XD level with 6-311++G(2d.2p) basis sets.

The shielding constant of the C atom of the small cage was lower than that of the large cluster consisted of the small cage and the 12 neighboring large cages. The charge of the methane molecule of the small cage was -1.47 e while that of the large cluster was -0.19 e. The DFT calculation for methane hydrate crystal was performed under the periodic boundary condition and the estimated charge of the methane molecule in the small cage was -0.15e. The underestimation of the shielding constant of the small cage will be related to the overestimation of the charge of the methane molecule.

1) M.J. Frisch, et al. Gaussian 16, Revision B.02, Gaussian, Inc., Wallingford, CT, 2016.

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Freezing-Induced Acidity Change: Mechanisms and their Possible Impacts on Polar Chemistry

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The acidity of sea ice and snow plays a key role in the chemistry of the cryosphere. Several reactions are either accelerated or allowed by acidic environments[1, 2]. A number of studies have shown that the acidity of frozen samples differs from the bulk acidity in the liquid state. Regrettably, the mechanisms of acidification or acidity changes in general have not been detailed sufficiently to date.

In artificial sea water, we detected three main freezing-induced effects, including a) Workman-Reynolds[3], b) freeze-concentration [4], and c) mineral crystallization[5]. The items are ordered by the overall importance. The obtained knowledge facilitated explaining successfully the freezing-induced acidification of the relatively complicated system of seawater. We utilized spectroscopic acid-base indicators and measured their spectra in ice matrices; this step then allowed us to observe the environment where nearly all the chemicals reside, namely, the ice veins. The results showed that the natural source of acidity arising from sea ice is sufficient to facilitate several environmentally relevant reactions.

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Spectroscopic and Microscopic Study of Freeze-Concentrated Solutions

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The freezing of aqueous solutions causes water segregation in ice crystals and freeze-concentrated solutions (FCSs), namely, in the contaminated veins, where a significant, concentration increase-induced aggregation takes place [1, 2]. Aggregation is a fundamental process in chemistry, with molecules associating to form larger structures, commonly referred to as aggregates. This effect occurs through various mechanisms, such as van der Waals forces and electrostatic interactions [3]. We report on the freezing-enhanced aggregation of methylene blue with respect to the concentration of inorganic salts (NaCl, $MgCl_2$ and $CaCl_2$) and sugars (sucrose and glucose).

Our samples were analyzed via UV-Vis spectroscopy to examine the enhanced aggregation on molecular level and by means of environmental scanning microscopy to inspect the inner ice structures and contaminants.

We detail the impact of the cooling rates and salt/sugar concentration, proposing that a low concentration or slow rates lead to a several orders of magnitude higher degree of aggregation than a high concentration or high rates. These results are rationalized by differences in the specific surface areas revealed via microscopic images. Furthermore, we observed vitrification and a subsequent cold crystallization of NaCl freeze-concentrated solutions, the latter being associated with major aggregation changes.

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Exploring the Impact of the Ice Matrix on the Photophysical Behavior of Phenolic Compounds

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Phenolic compounds have garnered significant attention in recent decades due to their harmful effects on human health and the environment. Their low reactivity and inability to undergo direct photolysis results in widespread distribution and accumulation of phenols in the environment [1]. The reactivity is, however, strongly influenced by various factors, such as the temperature, ionic strength [2] or phase transition [3].

To evaluate the behavior of phenols under various conditions, we utilize UV-Vis and fluorescence spectroscopies. The frozen samples, prepared at environmentally relevant temperatures, exhibit a small bathochromic shift and broadening of their absorption peaks. Although these changes may seem rather insignificant, they have a potential to enable or accelerate phenol photolysis in tropospheric conditions. Below the eutectic point temperature, liquid veins solidify, and the phenol crystal is formed. We have investigated the photophysical properties of the crystals, using diffuse reflectance and fluorescence spectroscopy because the properties and reactivity may differ from those of the solution.

High ionic strength (up to 20 M) was used to prepare the liquid samples as a model system for the highly concentrated solution in the ice veins. We show the impact of several salts at varied concentrations on the acid-base equilibrium and the consequent photophysical properties of phenols.

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Session numbers **in bold** show presenters.

Sapporo Town Map Around the Conference Hall of Hokkaido Univ.