France-Japan CREST Workshop on Nanomechanics

13-15　November 2024

Laboratory of Tribology and Dynamics of Systems (LTDS),
Ecole centrale de Lyon, France

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France-Japan CREST Workshop on Nanomechanics, Multiscale Mechanics and Tribology

Date : 13th-15th of November 2024
Venue : Amphitheater 1, Laboratory of Tribology and Dynamics of Systems (LTDS)
Ecole centrale de Lyon, France

Organizers:

Kohzo Ito (Research Center for Macromolecules and Biomaterials, National Institute for Materials Science/Graduate School of Frontier Sciences, The University of Tokyo)
Kazue Kurihara (NICHe, Tohoku University)
Denis Mazuyer (LTDS, Ecole Centrale de Lyon)
Masashi Mizukami (NICHe, Tohoku University)
Juliette Cayer Barrioz (LTDS, Ecole Centrale de Lyon)
Vincent Fridrici (LTDS, Ecole Centrale de Lyon)

Host:

Agence nationale de la recherche (ANR), France
Ecole Centrale de Lyon (ECL)
Tohoku University
ELyT (Engineering and Science Lyon Tohoku) Global
Universite de Lyon
Centre national de la recherche scientifique (CNRS)
Japan Science and Technology Agency (JST), Japan

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Date : 13th-15th of Nov. 2024
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Program

Wednesday 13th of November 2024

10:00 Opening remarks
CREST nanomechanics at JST, Kohzo Ito
(Research Center for Macromolecules and Biomaterials, National Institute for Materials Science/Graduate School of Frontier Sciences, The University of Tokyo)

10:10 Kohzo Ito (Research Center for Macromolecules and Biomaterials, National Institute for Materials Science/Graduate School of Frontier Sciences, The University of Tokyo)
"Introduction of Slide-Ring Materials for Circular Economy"

Masashi Mizukami (Tohoku University)
"Multi-scale elucidation of friction mechanisms in ice-rubber interfaces: Nano approach"

Denis Mazuyer (LTDS, Ecole centrale de Lyon)
"Elucidation of friction mechanisms in water-rubber multi-asperity interfaces"

12:00 *Lunch*

13:30 Daniel Nelias (LaMCoS, INSA Lyon)
"Fatigue of materials, a few ideas to go further, faster: ultrasonic testing"

Katsuhiro Tsunoda (Bridgestone)
"Quantifying the Enhancement Effect of Strain Induced Crystallization on Tearing Energy by Edge Crack Test Method"

Pierre-Emmanuel Mazeran (UTC)
"A unique nanotribology platform"

Eric Berge (Michelin)
"Michelin, Tire Grip on Ice"

15.30 Coffee break and LTDS visit

Banquet

Thursday 14th of November 2024

9:00 Koshi Adachi (Tohoku University)
"Creation of continuous ultra-low friction interface by controlling concerted tribochemical reaction and construction of design concept for long-term reliable mechanical systems"

Li Fu (LTDS, Ecole centrale de Lyon)
"Inverse design strategies for textured surfaces: achieving targeted friction laws"

Yuji Kinose (Kyoto University)
"Hierarchical understanding and controlling the wear phenomena of ultralow-friction polymer brushes"

10:30 *Coffee break*

11:00 Julien Scheibert (LTDS, Ecole centrale de Lyon)
"Designing Metainterfaces with Specified Friction laws"

Koichi Mayumi (The University of Tokyo)
"Tough Polymer Gels Reinforced by Strain-Induced Crystallization"

Gaylord Guillonneau (LTDS, Ecole centrale de Lyon)
"Surface mechanical properties and metallurgical evolutions along temperature ramp by High Temperature Scanning Indentation"

12:30 *Lunch*

14:00 Jun Yamamoto (Kyoto University)
"Fluctuation Microscopy"

Juliette Cayer Barrioz (LTDS, Ecole centrale de Lyon)
"Squeeze and nanomechanics of adsorbed boundary layers in a lubricated interface"

Ken Nakano (Yokohama National University)
"Abnormal Stribeck Curves of Concentrated Polymer Brushes in Macro and Nanoscales"

15:30 *Coffee break*

16:00 Short presentations of young participants
Anderson Kaiser (LTDS, Ecole centrale de Lyon)
"In situ Analysis of a Rubber/Ice Interface"

Michael Stevens (Tohoku University)
"Investigating the viscoelastic properties of the rubber-ice interface using the low temperature surface force apparatus"

Yutaka Takahashi (Tohoku University)
"Effect of Hyperbranched Polymers as Additive on Lubrication Properties of Base Oil"

Antoine Mille (LTDS, Ecole centrale de Lyon)
"Evolution of stress/displacement fields and contact area of PDMS sphere during oblique loading and shearing"

Yixin Su (Tohoku University)
"Interfacial Friction in Carbon Nanotubes (CNTs)/Ceramics Composites: A ReaxFF Study to Reveal CNT Reinforcing Mechanisms"

Ikki Yasuda (Keio University)
"In-layer inhomogeneity of molecular dynamics in quasi-liquid layers of ice"

Takumi Sato (Keio University)
"Molecular Simula-on of Fric-on Phenomena at the Ice-Polymer Interface"

Mizuho Yokoi (Tohoku University)
"Fracture and Degradation Mechanisms in Nitrided Steel Surface through Reactive Molecular Dynamics Simulations"

18:30 *End of the day / Dinner on your own*

Friday 15th of November 2024

9:00 Kazue Kurihara (Tohoku University)
"Confined Liquids Studied by Resonance Shear Measurement：
Molecular Mechanism of Lubrication"

Vincent Fridrici (LTDS, Ecole centrale de Lyon)
"Multiscale analysis of the tribological behavior of polymer-based composite in contact with steel under grease lubrication: from nanoscale tribofilms to macroscale damage"

Kenji Yasuoka (Keio University)
"Molecular simulation and machine learning for friction mechanism"

Davy Dalmas (LTDS, Ecole centrale de Lyon)
"In situ X-ray computed tomography study of a sphere/plane contact under normal and shear loadings"

11:00 Closing remarks

Wednesday 13th of November 2024

Introduction of CREST Nanomechanics and Slide-Ring Materials for Circular Economy

Kohzo Ito*

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National Indtitute for Materials Science, Sengen, Tsukuba, Ibaraki 305-0047 Japan

CREST stands for "Core Research for Evolutional Science and Technology." It is one of major programs by Japan Science and Technology Agency (JST) that aims to support innovative and pioneering research in various scientific and technological fields. In the research area of Nanomechanics, we aim to connect the macroscopic mechanical properties and nanoscale atomic or molecular dynamics to find the governing factors that determine the mechanical properties on the macroscale and to elucidate the mechanisms of their actions in nano or meso scale, and to find a principle or establish a guideline to yield innovative materials with new mechanical properties.

We have developed the Slide-Ring (SR) materials with polyrotaxane (PR), in which polymer chains are topologically interlocked by figure-of-eight cross-links. Recently, we have reported the stretch induced crystallization of the SR gel, which leads to extremely high toughness and recoverability. And we have found that PR drastically improved the mechanical properties, self-healing, chemical decomposition, and marine biogegradability of vitrimers. These findings may lead to the development of environment-friendly plastics that exhibit most of the properties required for a circular economy.

Professor Kohzo Ito

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Major Fields: Polymer Science, Supramolecular Chemistry

Biography: Kohzo Ito is a University Professor at The University of Tokyo and a fellow at National Institute for Materials Science. He received his B. E, M. E. and Ph. D. degrees in applied physics from The University of Tokyo. In 1986, he joined the Research Institute of Polymers and Textiles. He was transferred back to Faculty of Engineering, the University of Tokyo in 1991 and promoted to full professor at Graduate School of Frontier Sciences, the University of Tokyo in 2003. He is now the president of the Society of Polymer Science, Japan, and is running big national projects as a program director (SIP) and project manager (Moonshot Program). He has been researching the polymer physics and supramolecular chemistry, and now is focusing on polyrotaxane using cyclodextrin, necklace-like supramolecule with topological characteristics. He invented slide-ring materials with movable cross-links by cross-linking polyrotaxane in 2000, and set up a venture company to urge the application of the slide-ring materials in 2005. He has been the author of over 300 publications including original research papers, reviews, and books, and about 70 patents. He received The Award of the Society of Polymer Science, Japan (2006). And he is currently an editor of Polymer, Elsevir.

Main Publications

1. Yasushi Okumura and Kohzo Ito; “The polyrotaxane gel: a topological gel by figure-of-eight cross-links”, Advanced Materials, **13(7)**, 485-487(2001).
2. Chang Liu, Naoya Morimoto, Lan Jiang, Sohei Kawahara, Takako Noritomi, Hideaki Yokoyama, Koichi Mayumi, Kohzo Ito, ”Tough hydrogels with rapid-reinforcement”, Science, 372(6546), 1078-1081 (2021).
3. Shota Ando, Masaki Hirano, Lisa Wakatabe, Hideaki Yokoyama, Kohzo Ito, “Environment-friendly sustainable thermoset vitrimer-containing polyrotaxane”, ACS Materials Letter, 5, 3156-3160 (2023).

Multi-scale elucidation of friction mechanisms in ice-rubber interfaces: Nano approach

Masashi Mizukami
New Industry Creation Hatchery Center, Tohoku University, Sendai, 980-8577, Japan

Driving on a frozen roads are slippery, which reduces the safety of driving. In order to improve grip of tire on ice, an increasing interest to the interaction between ice and rubber has emerged. However, ice-rubber friction is governed by multiple factors, such as melting and premelting of ice, rubber viscoelasticity etc., and the understanding of its mechanism has been remained as a quite difficult issue. In our CREST project, we employ a combination of nanoscopic approach by Tohoku and macroscopic approach by Lyon, and simulation approach by Keio for understanding friction mechanism of ice-rubber interfaces.

In this presentation, we will show new insights on the friction of ice obtained by our nanoscopic approach using low temperature surface forces apparatus (LowT-SFA, Fig.1).[1, 2 3] The formation of a liquid-like water layer even below the bulk melting point of ice, so called ice premelting, has been recognized recently, and this phenomenon can explain the low friction at conditions of low contact pressure and low sliding speed. However, premelting is mainly known for the surfaces of ice in contact with a gaseous phase.

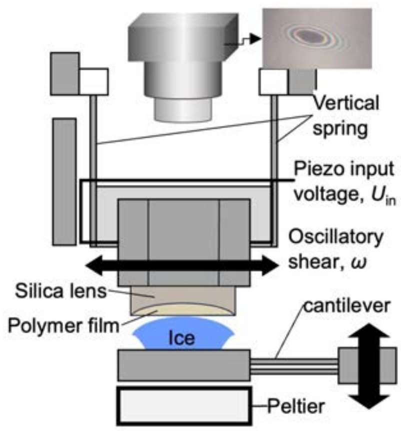

Fig.1 Schematic of the apparatus used for studying ice-polymer interfaces.

In this study, we investigated interfaces between ice and polymer films with various hydrophilicity (polystyrene (PS) and polyvinylalcoholu (PVA)) using a LowT-SFA.[4] At the contact interface of ice-PS, the area remained almost constant (Fig.2(a)). On the other hand, for the ice-PVA, the contact area gradually increased at temperatures above ca.-10 ℃, then drastically increased at temperatures above -5 ℃ (Fig.2(b)). The increase in the contact zones was associated with a liquid-like motion. These results clearly showed that the contact of PVA surface significantly enhance the premelting behavior. Interestingly, the enhanced premelting was not observed for the ice in contact with mica as well as silica surfaces although they are more hydrophilic compared with PVA film. Therefore, the enhanced premelting observed for ice in contact with a PVA film could be ascribed to the mobility of the polymer chain.

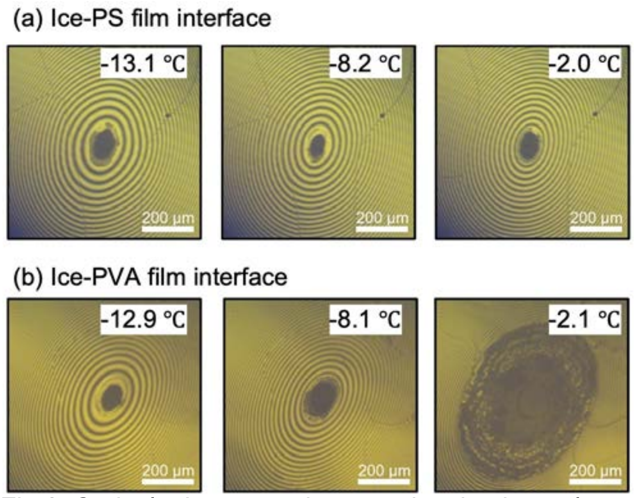

Fig.2 Optical microscope images showing ice-polymer film contact zones at different temperatures. (a) Ice-PS film interface, (b) Ice-PVA film interface.

Reference
1. F. Lecadre, M. Kasuya, A. Harano, Y. Kanno and K. Kurihara, *Langmuir*, 2018, **34**, 11311-11315.
2. F. Lecadre, M. Kasuya, Y. Kanno and K. Kurihara, *Langmuir*, 2019, **35**, 15729-15733.
3. F. Lecadre, M. Kasuya, S. Hemette, A. Harano, Y. Kanno and K. Kurihara, *Soft Matter*, 2020, **16**, 8677-8682.
4. J. Pallbo, S. Hemette, M. Mizukami and K. Kurihara, *Chem. Lett.*, 2024, **53**, 50.

Associate Professor Masashi Mizukami

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Major Fields: Surface forces measurement, Nano-tribology, Colloid & Interface Science

Biography:

1999	PhD (Engineering), Department of Applied Physics (Nagoya University)
1999-2001	Post doctral fellow, ICRS (Tohoku University)
2001-2003	Assistant Professor, ICRS (Tohoku University)
2003-2008	Assistant Professor, IMRAM (Tohoku University)
2008-2013	Lecturer, IMRAM (Tohoku University)
2013-2020	Associate Professor, IMRAM (Tohoku University)
2020-	Associate Professor, NICHe (Tohoku University)

Main Publications

1) M. Mizukami, M. Moteki, K. Kurihara, Hydrogen-Bonded Macrocluster Formation of Ethanol on Silica Surfaces in Cyclohexane, *J. Ame. Chem. Soc.*, **124**, 12889–12897 (2002).
2) K. Tomita, M. Mizukami, S. Nakano, N. Ohta, N. Yagi, and K. Kurihara."X-Ray Diffraction and Resonance Shear Measurement on Nano-Confined Ionic Liquids", *Phys. Chem. Chem. Phys.*, **20**, 13714-13721 (2018).
3) M. Mizukami, H.-Y. Ren, H. Furukawa, K. Kurihara, "Deformation of Contacting Interface between Polymer Hydrogel and Silica Sphere Studied by Resonance Shear Measurement", *J. Chem. Phys.*, **149**, 163327 (2018).
4) M. Mizukami, N. Ohta, K. Tomita, T. Yanagimachi, Y. Shibuya, N. Yagi, K. Kurihara, "Effects of Surface and Shear Forces on Nano-confined Smectic-A Liquid Crystals Studied by X-ray Diffraction", *Phys. Chem. Chem. Phys.*, **23**, 131-138 (2021).
5) M. Mizukami, T. Yanagimachi, N. Ohta, Y. Shibuya, N. Yagi, K. Kurihara, "Structures of Nanoconfined Liquids Determined by Synchrotron X-ray Diffraction", *Langmuir*, **38**, 5248-5256 (2022).

Elucidation of Friction Mechanisms in Water-Rubber Multi-Asperity Interfaces

D. Mazuyer
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Institut Universitaire de France

Many mechanical systems involve water-rubber interfaces such as joints sealing, tire/road or wiper blade/windscreen contacts. Their friction mechanisms rise from the combining three major sources which relative contribution depends on the environment of the contact and on the water phases:

- The proper viscoelastic dissipation of the rubber itself;
- The adhesive nature of the contact which is governed both by the molecular structure and the surfaces roughness;
- The dynamics of the multi-asperity interface.

In this framework, the challenge is the investigation of the water-rubber interfaces over a macroscopic scale that covers a sufficient amount of contact spots in order to develop a statistical approach. In this talk, the latter is highlighted through two particular examples:

- The stick-slip of an elastomer/glass contact immersed in liquid water: thanks to a model, based on a single degree-of-freedom mass-spring-damper oscillator we defined a stability criterion combining on the elastomer intrinsic material damping and the friction-velocity dependence. The origin of the instability is explained the physical nature of the contact spots in which we pointed out the prime importance of adhesion capillary forces. A friction law based on the surface topography analysis of the rubber was established;
- The unexpected coupling between adhesion, elastomer viscoelasticity and thermal effects in the frictional behavior of an ice/rubber contact: thanks to a in situ contact area measurements, a dimensionless friction master curve was obtained with the sliding velocity, regardless of the temperature and the material properties. A predictive friction model was proposed to explain the bell-shape friction-velocity curve for which the classical WLF transform is not relevant.

Professor Denis Mazuyer

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Major Fields:

- Ultra-thin film lubrication and friction
- Surface engineering in tribology
- Multi-scale advanced tribology experimentation

Biography: Denis Mazuyer, is an engineer from École Centrale de Lyon (1986), holds a PhD in mechanics (1989) under the supervision of Prof. Jean-Marie Georges. He was graduated in mathematics in 1991 and he obtained the habilitation to supervise research in 1995. Recruited in 1989 as a research fellow at the CNRS, he was promoted as a full Professor at the École Centrale de Lyon in 2000. He carries out his research on the tribology of thin-film lubricated interfaces and the surface effects on friction at the Laboratoire de Tribologie et Dynamique des Systèmes (LTDS), which he led between 2007 and 2015. He was awarded the prize for the best external research awarded by SOLVAY in 2000 and the Edmond Prize Bisson of the Society of Tribologists and Lubrication Engineers (STLE) in 2009. He is co-author of 108 international publications and holds four patents. He has been Chairman of the École Centrale de Lyon's Restricted Board from 2013 to 2017. He also chaired the GIE Manutech-USD, which develops and operates equipment of excellence on surface texturing processes, from 2012 to 2018. He is a senior member of Institut Universitaire de France since 2024.

Main Publications

1. J. Baudry, E. Charlaix, A. Tonck, D. Mazuyer, "Experimental evidence for a large slip effect at a nonwetting fluid− solid interface", Langmuir 17 (17) pp. 5232 – 5236, 2001.
2. L. Mourier, D. Mazuyer, F.-P. Ninove, A.A. Lubrecht, "Lubrication mechanisms with laser-surface-textured surfaces in elastohydrodynamic", Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology, 224(8): 697–711 (15 pages), 2010.
3. L. Frérot, A. Crespo, J.A. El-Awady, M.O. Robbins, J. Cayer-Barrioz, D. Mazuyer, "From Molecular to Multiasperity Contacts: How Roughness Bridges the Friction Scale Gap", ACS Nano, 17(3), pp. 2205 – 2211 (7 pages), 2023

Fatigue of materials, a few ideas to go further, faster: ultrasonic testing

Daniel Nélias[1]

1. INSA Lyon, CNRS, LaMCoS, UMR5259, 69621 Villeurbanne, France

One of the key challenges for the planet to last longer is to design materials for ever. Of course this is not realistic. No one can certify it, humans and devices have all a deadline.

At our engineering level, the goal is to design a material for a given application that will last billions of cycles, if possible. The presentation will focus on the fatigue of high-performance steels at low load – elastically speaking – and high number of cycles. As introduction an original test rig will be described and some results presented. The main focus is on rolling contact fatigue.

by Yukitaka Murakami, 2017

Professor Daniel Nélias

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Major Fields: Contact Mechanics, Rolling Contact Fatigue, Surface Treatments

Biography: Daniel Nélias is Professor of Mechanical Engineering at INSA Lyon. His research deals with contact mechanics (effect of plasticity and inhomogeneities on running-in, rolling contact fatigue or fretting wear, viscoelastic layered materials), the characterization of materials at high temperature or after high rate thermal loading, the modelling of processes including surface treatment (shot and laser peening, cavitation and water peening, electromagnetic pulse peening, grinding, cutting, welding, coating deposit, cold spray and additive manufacturing) and integrity of structures under extreme conditions.

Main Publications

1. Nélias, D, Dumont, ML, Champiot, F, Vincent, A, Girodin, D, Fougères, R, Flamand, L (1999) 'Role of inclusions, surface roughness and operating conditions on rolling contact fatigue', *Journal of Tribology* **121** (2), 240-251 10.1115/1.2833927
2. Jacq, C, Nélias, D, Lormand, G, Girodin, D (2002) 'Development of a three-dimensional semi-analytical elastic-plastic contact code', *Journal of Tribology* **124** (4), 653-667 10.1115/1.1467920
3. Bardel, D., Perez, M., Nelias, D., Deschamps, A., Hutchinson, C. R., Maisonnette, D., Chaise, T., Gamier, J., Bourlier, F. (2014) 'Coupled precipitation and yield strength modelling for non-isothermal treatments of a 6061 aluminium alloy', *Acta Materialia* **62**, 129-140 10.1016/j.actamat.2013.09.041
4. Koumi, Koffi Espoir, Zhao, Lv, Leroux, Julien, Chaise, Thibaut, Nelias, Daniel (2014) 'Contact analysis in the presence of an ellipsoidal inhomogeneity within a half space', *International Journal of Solids and Structures* **51** (6), 1390-1402 10.1016/j.ijsolstr.2013.12.035

Quantifying the Enhancement Effect of Strain Induced Crystallization on Tearing Energy by Edge Crack Test Method

K. Tsunoda[1], K. Urayama[2]

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2. Kyoto University, Kyotodaigaku-Katsura, Nishikyo-Ku, Kyoto 615-8510, Japan

Natural rubber (NR, cis 1-4, polyisoprene) is commonly adopted bio-sourced polymer in rubber industry. NR exhibits strain induced crystallization (SIC) resulting in superior mechanical properties, compared to other synthetic rubbers. The fracture strength of rubber can be described utilizing tearing energy (G) and G is strongly associated with viscoelastic energy dissipation. The mechanical strength of SIC rubber, like NR, is governed by not only the viscoelastic energy dissipation but also the SIC enhancement effect. Experimentally measured G for SIC rubber includes the contributions of these two components, resulting from viscoelastic energy dissipation (G_{-VE}) and SIC (G_{-SIC}). Importantly, G_{-SIC} has a threshold concerning its onset, dependent on strain-rate and ambient temperature. This is because SIC is fundamentally a kinetic process driven by crystallization. Quantitative determination of G_{-SIC} and its threshold condition to be generated is clearly important for engineering application but this was not fully investigated. We've developed a methodology to quantify the G_{-SIC} within the experimentally measured G and also determine the threshold conditions for the onset of the SIC effect with focusing on the unique rupture mode transition in single-side pre-notched tensile specimen (edge crack test). In this presentation, detailed theoretical background, experimental methodologies, and effect of nano-micro-macro polymer structure for G_{-SIC} and its onset will be reported.

Dr. Katsuhiko TSUNODA

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Major Fields: Fracture mechanics, Rubber physics

Biography:

Katsuhiko Tsunoda jointed Bridgestone corporation in 1991 and started his carrier as material researcher for non-tire products, like rubber truck, conveyor belts and automotive hoses.
From 1998, he studied fracture mechanics of rubber under the direct supervision of Prof. Alan Thomas at Queen Mary, University of London and completed Ph.D. in 2001.
From 2011, he was transferred to central research division and working materials science research field.
During 2014 to 2019, he jointed ImPACT research program as project leader challenging innovative tough rubber compound development. From 2020, he jointed CREST nano mechanics and is researching strain induced crystallization.

Main Publications

K. Tsunoda & K. Urayama, Soft Matter, 19, 1966 (2023)
K. Tsunoda, et. al., Journal of Material Science, 35, 5187 (2000)
J. Busfield, K. Tsunoda, C.K.L. Davies, A.G. Thomas, Rubber Chem. And Technol., 75(4), 643 (2002)

A unique nanotribology platform

C. De Sousa[1], P-E. Mazeran[1], O. Noel[2].

1. Université de technologie de Compiègne, CNRS, Roberval (Mechanics energy and electricity), Centre de recherche Royallieu - CS 60 319 - 60 203 Compiègne Cedex

2. Institut des Molécules et Matériaux du Mans, Université du Maine, UMR CNRS 6283, Avenue Olivier Messiaen, Cedex 9, 72085, Le Mans, France

We have developed a unique platform for nanotribology investigations, using an Atomic Force Microscope, transformed in a nanotribometer. This platform is based on three original aspects:

- A homemade V-shape LFM caliber [1], Using the wedge method, it allows us to caliber the lateral force quickly and accurately.
- The circular mode [2], that consist in coupling a high frequency circular displacement to a force spectrum. Allowing the instantaneous measurement of the friction law.
- The Initiation of sliding mode [3], that consist in a lateral oscillating displacement of increasing then decreasing amplitude, allowing the study of the transition between static and dynamic friction.

The presentation will focus on these three aspects and will provide few results based on application examples.

[1] Mazeran et al., Atomic Force Microscopy lateral force calibration using a V-shape sample, submitted to Review of Scientific Instruments (Sept. 2024).

[2] Nasrallah et al., Circular mode: A new scanning probe microscopy method for investigating surface properties at constant and continuous scanning velocities. 82 (2011) 113703

[3] Mazeran, Beyaoui, Initiation of Sliding of an Elastic Contact at a Nanometer Scale Under a Scanning Force Microscope Probe, 30-1 (2008) 1-11

Pierre-Emmanuel MAZERAN

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Major Fields: Nanotribology, Atomic Force Microscopy, Friction, adhesion and wear at the nanoscale, Nanoindentation

Biography: In order to better understand the elementary phenomena responsible for friction and the laws governing them, we study the tribological behavior of contacts at the nanoscale. The originality of our work lies in transforming an Atomic Force Microscope into a fast and functional nanotribometer by studying the response of a contact subjected to harmonic displacements.

The circular mode involves moving the contact in a circular motion while varying the normal force. It allows for instant measurement of the friction law and shows influence of sliding velocity on adhesion. The initiation of sliding mode consists of moving the contact with an increasing displacement amplitude. It allows for observing the transition between static and dynamic friction and studying the influence of sliding velocity speed on the friction force.

Finally, we developed a method for calibrating the lateral force signal in Atomic Force Microscopy. The principle involves using the Wedge method with a sample featuring a V-shaped scratch, where the surfaces have large areas with the same slope and friction coefficient. This allows for the acquisition of very high-quality data, enabling particularly robust calibration.

Main Publications

1. H. Nasrallah, P.-E., Mazeran, O. Noël, O., "Circular mode: A new scanning probe microscopy method for investigating surface properties at constant and continuous scanning velocities", Review of Scientific Instruments, 82 (11), (2011) art. no. 113703.
2. Mazeran, P.-E., Beyaoui, M., Initiation of sliding of an elastic contact under a Scanning Force Microscope probe, Tribology Letters, 30-1 (2008) 1-11
3. O. Noël, P.-E. Mazeran, H. Nasrallah, "Sliding velocity dependence of adhesion in a nanometer-sized contact", Physical Review Letters, 108 (1), (2012) art. no. 015503.

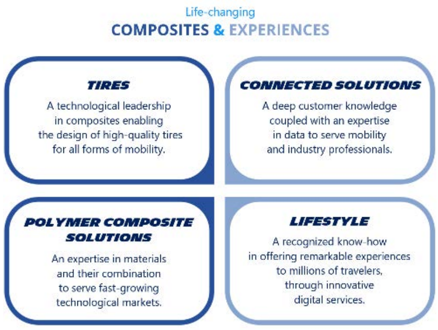
Michelin, Tire Grip on Ice

Eric Berger[1,*]
Yuji Kanno[1]
1. Manufacture Français des Pneumatique Michelin, 23 Place des Carmes Déchaux, 63000 Clermont-Ferrand, France

This presentation aims to present Michelin group and why Michelin needs academic partners to provide better mobility to our customers.

Michelin Group

Michelin Group employs 132,500 people worldwide, of which around 6,000 work in the area of research and development, and spends €1.2 billion per a year on innovation. 86 production sites locate worldwide, includes 45 high-tech materials production facility. And we are also, of course, committed to reducing CO_2 emission and environmental impact for the stake of the environment.

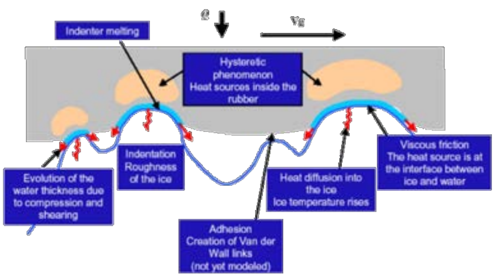


Our main activities now include four main area, with two keywords. They are "composites" and "experience". In the first area, tire, we aim to develop and provide high quality tires for all forms of mobility though technology leadership in composites. The second area is polymer composite solutions. We aim to bring our accumulated technologies and expertise in polymers and composites to current and growing technically challenging markets. The third area is connected solution, where the recent remarkable development of IT technology has made it easy to access tire usage and operating conditions along a lot of complemental information. We aim to provide better mobility to our customers by using these vast amounts of data and our analysis capabilities based on expertise to propose better tire and its maintenance. The last area is lifestyle. Through the Michelin Red Guide and other guidebooks, we aim to offer an irreplaceable experience.

Winter Grip and Tribology

For the mobility on the winter road, Michelin offers 3 types of tires for winter road. 1st category is Nordic tire which provide the best performance on severe winter road condition. These tires give us the best grip performance on ice- and snow-covered road and we offer in North America, Japan, Nordic countries and China where road is covered by ice and snow in winter. 2nd category is Alpin tires. This tire provides the better performance on winter road and on the road covered by water, or dry condition. We offer these tires mainly in Western Europe counties where the demands for both winter and summer grip performance is high because of driving style, road conditions in these countries. The last category for tires on winter road is all season tire. We offer these tires mainly in United State, Western Europe counties where severity of winter road is not high and from the demands from customers. To offer better mobility on the winter conditions, it is necessary to understand how road conditions are severe in winter, how customers want to use their vehicles and tires and how they drive vehicles. This is the reason why Michelin has R&D centers locates around the world and close to customers and markets.

Stopping, braking on the icy, snowy road is also multiscale and Multiphysics problem, when the brakes are applied strongly on ice covered road, at the vehicle scale, Antilock Braking System works and it results in a variety of relative speeds between tire surface and ground. At the same time due to vehicle dynamics, vertical load on a tire changes. At the tire alone scale, tire is deformed by load, it then forms a contact surface to the ground. At the scale of a tread block, this tread block also deforms according to the load applied to it, and deformation of each tread block is not same in a contact patch due to tire kinematics such as rotation and deformation. And at the material scale, it is the one of the key scale to generate grip forces thanks to visco-elasticity of rubber material and cyclic indentation from ground due to sliding. at molecular scale, each ingredient and formulation of a material defines its viscoelastic properties. To understand mechanisms and physics at each scales, we use experimental tools, models and simulations tools adapted to each scale.



When focusing on grip on ice, there are several phenomena, physics happens dynamically. When rubber contact to ice and slide in tangential direction, at the begging we can assume that rubber contact to ice surface directly and it generates friction force by viscoelasticity of rubber and adhesion force between rubber and ice. After a certain time of sliding, due to the heat generation by the friction force, the ice starts to melt at the interface and it evolves over time and generates water. These phenomena results in reduction of friction force and low friction coefficient on ice road. We could find several mechanism, viscoelastic dissipation, adhesion between ice and rubber, hydrodynamics with water generated by the frictional heat. And this is done dynamically when tire rolls on ice at each tread block and each surface of rubber. For the understanding of mechanisms and phenomena, it is necessary to have an understanding of the problem with multiscale tribological analysis.

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Tire Performance Expert: Contact (Wear and Grip)

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Major Fields: tire, grip, wear, tribology, contact physics, finite element analysis,

Biography:

Main Publications

1.
2.
3.

Thursday 14th of November 2024

Creation of continuous ultra-low friction interface by controlling concerted tribochemicalreaction and construction of design concept for long-term reliable mechanical systems

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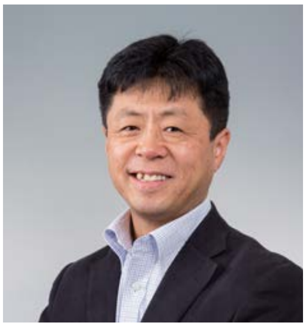
Ultra-low friction is recognized as one of key issues for high efficient usage of energy in mechanical systems. In addition, stability and durability of such ultra-low friction is a practically essential issue for real applications. To achieve it and its stability and durability, new materials, coatings, lubricants and new surface design have been strongly required in the world wide. In dry contact, boundary lubrication regime, mixed-lubrication regime except perfect hydrodynamic lubrication regime, friction surfaces at a stable stage always change significantly from the initial surface. That is to say, design concept for initial surface to control formation of friction interface at a stable stage is strongly required for further technology of ultra-low friction. On the other hand, it is well-known that beginning of sliding so-called running-in period is an important for stable friction by formation of well-conformed interface. In this presentation ultra-low friction obtained by using textured surface and carbon-based coatings under are mainly focused, and low friction technology is discussed from the view point of running-in.



Professor Koshi ADACHI

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Major Fields: Tribology

Biography:
Koshi Adachi graduated in Mechanical Engineering from Tohoku University in 1988 and obtained his Ph. D for research in Tribology from Tohoku University, Japan in 1998.

He started to work as a research associate in 1990, and he is currently full professor at the Faculty of Engineering, Tohoku University. He is the head of "Laboratory of Tribology and Nanointerface Engineering" and director of "Center for Tribologically-based Machine Design", in Division of Mechanical Engineering, Tohoku University.

His research interests span a wide range of tribology, including fundamental and application of tribology, with a particular interest in friction and wear mechanisms of advanced materials, technology for super-low friction such as surface texturing and new coatings, science and technology for running-in control and continuous formation of functional interface (nano-interface) during friction automatically, environmentally-friendly mechanical systems with water and gas lubrication, friction drive with ultrasonic and surface acoustic wave for precise positioning systems and control of tribo-chemical reaction. He is currently challenging to establish new concept named as "Tribologically-based Machine Design" and "Science of Running-in".

Main Publications

1. Kazuya Kuriyagawa, Koshi Adachi, Durability of Super-Low Friction of Hydrogenated Carbon Nitride Coatings in High-Vacuum Environment, Tribology Online, 19, 1 (2024) 62-73.
2. Yang Wang, Kentaro Hayashi, Yusuke Ootani, Shandan Bai, Tomomi Shimazaki, Yuji Higuchi, Nobuki Ozawa, Koshi Adachi, Maria-Isabel De Barros-Bouchet, Jean-Michel Martin, Momoji Kubo, Role of OH-termination in mitigating friction of diamond-like carbon under high load: a joint simulation and experimental study, Langmuir, 37 (2021) 6292-6300.
3. Kento Ihara, Koshi Adachi, Friction Reduction by Laser Irradiation for a Friction System Using Bearing Steel and Aluminum Alloy in Engine Oil, Tribology Online, 17, 4 (2022) 335-347.

Inverse design strategies for textured surfaces: achieving targeted friction laws

L.Fu, J.Scheibert

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The optimization of frictional interfaces is essential for various applications, such as touchscreens and robotic hands, where precise control over friction laws is paramount. While linear friction laws are commonly observed in natural surfaces, achieving such behavior in artificial surfaces with a limited number of asperities remains a complex challenge. This study introduces a systematic strategy for the inverse design of textured surfaces aimed at achieving linear friction laws, building upon the foundation provided by a discrete Greenwood-Williamson model, which initially resulted in an asymptotic friction law without a guaranteed intercept at zero [1].

Central to our approach is the employment of a genetic algorithm (GA) to optimize the heights of individual asperities, treating each asperity as an independent genetic unit. The application of GA allows us to efficiently explore and exploit the design space of asperity configurations. Our findings indicate that the optimal textured surface can be represented as a combination of a truncated exponential distribution and a demi-triangle distribution, effectively targeting the desired linear friction behavior. Moreover, this method showcases a remarkable flexibility, enabling the design of surfaces that can accommodate various friction laws, including both linear and non-linear configurations, while seamlessly addressing complex asperity geometries.

Through ongoing experimental validation on centimeter-scaled textured surfaces, we aim to establish this comprehensive and adaptable design approach for frictional interfaces, which is scale- and material-independent. This work paves the way for the development of energy-efficient, smart interfaces that meet a wide array of friction performance requirements, highlighting the transformative potential of genetic algorithms in surface design.

[1] A. Aymard, E. Delplanque, D. Dalmas, and J. Scheibert, Designing metainterfaces with specified friction laws, Science **383**, 200 (2024).

Professor Li FU

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Major Fields: AI for tribology, Surface engineering, Nanometric transport properties, Fluid-structure interaction

Biography:

Dr. Li Fu, assistant professor in the Laboratory of Tribology and Dynamics of Systems (LTDS) at Ecole Centrale de Lyon since 2022. He obtained his PhD in 2015 and subsequently held postdoctoral positions from 2016 to 2022. His research expertise lies at the intersection of tribology, surface engineering, and AI. He has made significant contributions to understanding friction mechanisms and applying AI methods to physical problems, in particular, he has coupled Reinforcement Learning techniques with real-world experiments to study the locomotion of robotic fish and optimize their swimming strategies.

Main Publications

1. Y. Xie*, L. Fu*, T. Niehaus, and L. Joly: Liquidsolid slip on charged walls: Dramatic impact of charge distribution, Physical Review Letters, (2020).
2. L. Fu, L. Joly and S. Merabia: Giant thermoelectric response of nanofluidic systems driven by water excess enthalpy, Physical Review Letters, (2019).
3. L. Fu, S. Merabia, and L. Joly: What controls thermo-osmosis? Molecular simulations show the critical role of interfacial hydrodynamics, Physical Review Letters, (2017).

Hierarchical understanding and controlling the wear phenomena of ultralow-friction polymer brushes

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The concentrated polymer brushes (CPBs), which have a graft density 1 order of magnitude higher than conventional polymer brushes (semi-dilute polymer brushes: SDPBs), take an elongated chain conformation almost comparable to their fully stretched one owing to mixing entropy with a good solvent. Therefore, CPBs exhibit unique properties, such as strong resistance against compression, distinctive size exclusion effect and ultra-low friction/good lubrication, different from those of SDPBs.[1] Among others, the CPBs with ultra-large film thicknesses of μm order demonstrated ultra-low friction/good lubrication properties even in a macroscopic contact, indicating the potential as a next-generation sliding material.[2]

The friction and lubrication mechanism of CPB can be understood by the Stribeck curve. In the regime of a high Stribeck number, CPB-modified substrates behave similarly to unmodified substrates, because the drag force of the lubricant is dominant as a hydrodynamic lubrication regime. As the Stribeck number decreases, the sliding system shifts to the mixed lubrication regime, and hence the friction increases. On CPB-modified substrates, the critical Stribeck number at which the system shifts to the mixed lubrication regime is lower than that on unmodified substrates, suggesting the expansion of hydrodynamic lubrication regime (by the contribution of an elastohydrodynamic lubrication specific to the swollen CPB system). In addition, the CPB system is characterized by the appearance of a shoulder in the hydrodynamic lubrication regime in the Stribeck curve, when a high load is applied. Because this shoulder become conspicuous with increasing load and lubricant viscosity, we consider that its origin is a viscoelastic response of a swollen CPB layer related to the pressure-dependent local viscosity.

It is important to elucidate the wear mechanism of CPB in order to use it as a next-generation sliding coating.[3-5] We performed a ball-on-disk test of CPB in a lubricant containing a fluorescent monomer with the aim of selective labeling of the wear point via polymerization of the fluorescent monomer from mechanoradicals generated by polymer-chain scission. We conducted the test using a partially scratched CPB sample to enhance the reproducibility of the onset of CPB wear. The fluorescent microscope image showed the wear marks uniformly located on the sliding tracks with low intensity and those growing from the scratch with high intensity (**Figure 1**). Based on these results, we propose a wear process consisting of two stage at a least: at an early stage of wear, the "random scission" of polymer chains occurs in CPB, and in the later stage, the accumulation of random scission triggers a "consecutive scission", leading to a "destructive wear" with a significant increase in friction coefficient. We are currently investigating the CPB design and sliding condition to suppress random and consecutive scission of polymer chains.

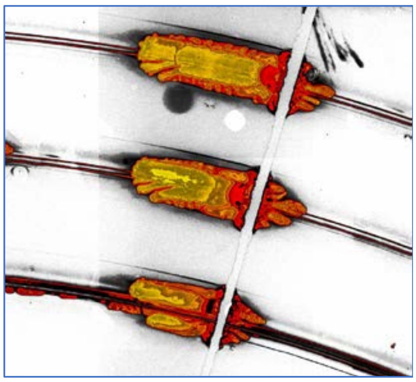
Figure 1. wear marks on CPB detected by fluorescence.

[1] Tsujii, Y. *et al. J. Phys. Conf. Ser.* **184**, 012031 (2009). [2] Sato, K. *et al. J Tribologi* **20**, 97-113 (2019).[3] Miyazaki, M. *et al. Wear* **482-483** (2021). [4] Vladescu, S. C. *et al. ACS Appl. Mater. Interfaces* **14**, 15818-15829 (2022). [5] Okubo, H., et al. *Langmuir* **39**, 18458-18465 (2023).

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Major Fields: Polymer Science

Biography:

Apr., 2009- May, 2013	Industrial Chemistry, Faculty of Engineering, Kyoto University
Apr., 2013- May, 2015	Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University (Master's Course)
Apr., 2015- May, 2018	Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University (Latter Doctoral Course)
Apr., 2018- Sep., 2020	Technical Assistant, Institute for Chemical Research, Kyoto University
Oct., 2020- Mar., 2021	Research Worker, Institute for Chemical Research, Kyoto University
Jun., 2021-	Assistant Professor, Research worker, Institute for Chemical Research, Kyoto University

Main Publications

1. Kinose, Y., Sakakibara, K., Ogawa, H. & Tsujii, Y. Main-Chain Stiffness of Cellulosic Bottlebrushes with Polystyrene Side Chains Introduced Regioselectively at the *O*-6 Position. *Macromolecules* **52**, 8733-8740 (2019).
2. Kinose, Y., Sakakibara, K. & Tsujii, Y. Conformational characteristics of regioselectively PEG/PS-grafted cellulosic bottlebrushes in solution: cross-sectional structure and main-chain stiffness. *Polym J* **54**, 503-513 (2022).
3. Kinose, Y., Sakakibara, K., Sato, O. & Tsujii, Y. Near-Zero Azimuthal Anchoring of Liquid Crystals Assisted by Viscoelastic Bottlebrush Polymers. *Acs Applied Polymer Materials* **3**, 2618-2625 (2021).

Designing metainterfaces with specified friction laws

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Many devices, including touchscreens and robotic hands, involve frictional contacts. Optimizing those devices requires fine control of the interface's friction law. We lack systematic methods to create dry contact interfaces whose frictional behaviour satisfies preset specifications. In this talk, I will present a generic surface design strategy to prepare dry rough interfaces that have predefined relationships between normal and friction forces [1]. Such metainterfaces circumvent the usual multiscale challenge of tribology [2], by considering simplified surface topographies as assemblies of spherical asperities. Optimizing the individual asperities' heights enables specific friction laws to be targeted. Through various centimeter-scaled elastomer-glass metainterfaces, I will illustrate different types of achievable friction laws, including linear laws with a specified friction coefficient and unusual non-linear laws. This design strategy represents a scale- and material-independent, chemical-free pathway toward energy-saving and adaptable smart interfaces.

[1] A. Aymard, E. Delplanque, D. Dalmas, J. Scheibert, *Science* **383**, 200-204 (2024)
[2] A. I. Vakis, *et al.*, *Tribology International* **125**, 169-199 (2018)

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Major Fields: Tribology ; Contact mechanics ; Interface design

Biography: A graduate of the Magistère de sciences de la matière at the École Normale Supérieure de Lyon and the Université Claude-Bernard Lyon-I, and agrégé de sciences physiques, Julien Scheibert obtained his doctorate in condensed matter physics from the Université Paris-VI in 2007. He is currently director of research at CNRS, within the Tribology and Systems Dynamics Laboratory (LTDS). His research interests lie at the interface between physics and mechanics, with the aim of establishing a quantitative link between experiments and modelling. His work has successively focused on :
- human tactile perception, and in particular the role of fingerprints in the perception of fine textures ;
- the rapid fracture of brittle heterogeneous solid materials ;
- the sliding dynamics of contact interfaces between rough solids.

Julien Scheibert has developed a recognised expertise in the contact mechanics of dry and rough interfaces, particularly for soft materials such as elastomers. He is now developing metainterfaces, the microstructure of which is optimised to provide tailor-made friction properties.

Main Publications

1. A. Aymard, E. Delplanque, D. Dalmas, J. Scheibert. Designing metainterfaces with specified friction laws. *Science* **383**, 200-204 (2024)
2. R. Sahli, G. Pallares, C. Ducottet, I.E. Ben Ali, S. Al Akhrass, M. Guibert, J. Scheibert. Evolution of real contact area under shear and the value of static friction of soft materials. *PNAS* **115**, 471-476 (2018)
3. J. Scheibert, S. Leurent, A. Prevost, G. Debrégeas. The role of fingerprints in the coding of tactile information probed with a biomimetic sensor. *Science* **323**, 1503-1506 (2009)

Tough Polymer Gels Reinforced by Strain-Induced Crystallization

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Tough polymer gels are required for various applications such as soft actuators/sensors, and artificial tendons/ligaments. For these applications, the polymer gels should show reversible mechanical responses under repeated high stress at a high frequency (ex. 1 Hz). Most tough hydrogels are reinforced by introducing sacrificial structures that can dissipate input energy [1, 2]. However, since the sacrificial damages cannot recover instantly, the toughness of these gels drops substantially during consecutive cyclic loadings. Recently, we have successfully developed tough and instantly recoverable polymer gels utilizing strain-induced crystallization (SIC) [3-6].

In order to realize SIC in polymer gels, the polymer chain orientation under stretching should be homogeneous. We have discovered that SIC occurs in slide-ring (SR) hydro and ion gels with slidable cross-links [3, 4], tri-branched PEG gels [5], and Tetra-branched PEG gels [6]. From in-situ wide-angle X-ray scattering (WAXS) experiments on the gels under repeated tensile deformation, we found that crystalline of PEG in the gels forms at a large strain and destructs quickly when applied stress is reduced (Fig.1). The reversible strain-induced crystallization yields the high toughness and instant recoverability.

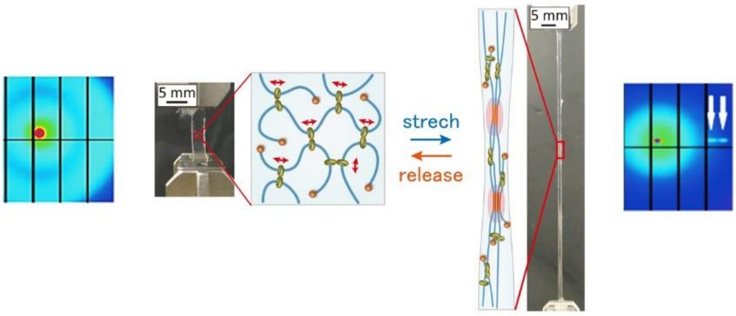

Fig.1 Reversible strain-induced crystallization of SR gels

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[4] K. Hashimoto, T. Shiwaku, H. Aoki, H. Yokoyama, K. Mayumi, K. Ito, Sci. Adv., 9, eadi8505 (2023).
[5] T. Fujiyabu, N. Sakumichi, T. Katashima, C. Liu, K. Mayumi, U. I. Chung, T. Sakai, Sci. Adv., 8, eabk0010 (2022).
[6] K. Hashimoto, T. Enoki, C. Liu, X. Li, T. Sakai, K. Mayumi, Macromolecules, 57, 1461 (2024).

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Major Fields: Polmer physics, Mechanical properties, Scattering techniques, Polymer networks

Biography:

2020.November–present

Associate Professor, Neutron Science Laboratory, The Institute for Solid State Physics, The University of Tokyo

2018.March–2020.October

Project Lecturer, Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo

2014.April–2018.February

Assistant Professor, Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo

2012.April–2014.March

Postdoctoral Fellow of Laboratoire SIMM/PPMD, ESPCI ParisTech

Main Publications

1. Kei Hashimoto, Takato Enoki, Chang Liu, Xiang Li,Takamasa Sakai, Koichi Mayumi*, "Strain-Induced Crystallization in Tetra-Branched Poly (ethylene glycol) Hydrogels with a Common Network Structure", Macromolecules, 57, 1461-1468 (2024).
2. Kei Hashimoto*, Toru Shiwaku, Hiroyuki Aoki, Hideaki Yokoyama, Koichi Mayumi*, Kohzo Ito *, "Strain-induced crystallization and phase separation used for fabricating a tough and stiff slide-ring solid polymer electrolyte", Science advances, 9, eadi8505 (2023).
3. Chang Liu, Naoya Morimoto, Lan Jiang, Sohei Kawahara, Takako Noritomi, Hideaki Yokoyama, Koichi Mayumi*, Kohzo Ito*, "Tough Hydrogels with Rapid Self-reinforcement", Science, 372, 1078-1081 (2021).

Surface mechanical properties and metallurgical evolutions along temperature ramp by High Temperature Scanning Indentation

G. Guillonneau[1)*], G. Tiphéne[1,2) *], P. Baral[3)], S. Comby-Dassonneville[4)], G. Kermouche[3)], J.M. Bergheau[1)], W.C. Oliver[5)], J.L. Loubet[1)].

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Increasing wear resistance of materials at high temperature is an important challenge to reduce energy losses. A thorough understanding of materials mechanical properties at the scale of tribological contacts is key. Thank to high temperature nanoindentation, measurements up to 1000°C are now feasible. Interpreting such data remains complicated since hardness can depend on microstructural evolutions occurring upon heating. A recent paper of Baral et al. [1] has highlighted the ability of high temperature nanoindentation to investigate in-situ microstructural evolutions in an aluminum alloy. However, usual high temperature nanoindentation methods are limited to the examination of processes whose evolutions are very slow.

A new technique, named High Temperature Scanning Indentation (HTSI), was developed, and allows for the measurement of surface mechanical properties by fast nanoindentations during a complete thermal cycle (i.e. during heating, holding at constant temperature, and cooling) [2]. This means the mechanical properties are measured continuously as a function of temperature during only one test, permitting earning time considerably. This method, first validated on a model material (fused silica), was then applied on different materials (metals, metallic glass, amorphous materials), the results showing the HTSI method is able to detect microstructural changes as a function of the temperature, through the mechanical properties variations [3,4]. In this workshop, the HTSI technique will be detailed, and some applications on different materials will be presented and discussed, in terms of mechanical properties and microstructure evolutions.

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Major Fields: micro-nanomechanics, tribolayers, extreme conditions

Biography:

I obtained my PhD in the field of nanomechanics at the Laboratory of Tribology and Systems Dynamics (LTDS) at Centrale Lyon in 2012. The subject concerned the improvement of nanoindentation technique in extreme conditions (temperature, extreme surface…). After my PhD thesis and a first post-doctoral internship at ENISE, LTDS, I spent 2 years in Switzerland doing a second post-doctoral internship in an EMPA laboratory (EMPA, Thun, Switzerland) in the field of micromechanics of materials in extreme conditions (developments of new micromechanical techniques to measure of surface mechanical properties at high temperature and high strain rate). I became associate professor at Centrale Lyon in 2015. I'm teaching mainly courses and practicals in materials engineering. I'm doing my research activity at the LTDS. My activity focuses on the understanding of mechanical properties of surfaces submitted to tribological solicitations.

Main Publications

1. G. Tiphéne, P. Baral, S. Comby-Dassonneville, G. Guillonneau, G. Kermouche, J.-M. Bergheau, W. Oliver, J.-L. Loubet, High-Temperature Scanning Indentation: A new method to investigate in situ metallurgical evolution along temperature ramps, J. Mater. Res. (2021). https://doi.org/10.1557/s43578-021-00107-7.
2. G. Guillonneau, M. Mieszala, J. Wehrs, J. Schwiedrzik, S. Grop, D. Frey, L. Philippe, J.-M. Breguet, J. Michler, J.M. Wheeler, Nanomechanical testing at high strain rates: New instrumentation for nanoindentation and microcompression, Mater. Des. 148 (2018) 39–48.

https://doi.org/10.1016/j.matdes.2018.03.050.

3. A. Dreano, S. Fouvry, G. Guillonneau, Understanding and formalization of the fretting-wear behavior of a cobalt-based alloy at high temperature, Wear 452–453 (2020) 203297. https://doi.org/10.1016/j.wear.2020.203297

Fluctuation Microscopy

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Conventional optical microscopes visualize static inhomogeneities such as orientation, concentration, and density within a material. *Fluctuation microscope* we have invented and developed is a revolutionary new microscope that can visualize "dynamic heterogeneity" which is the internal space-time structure of matter at the nano- to meso-scale, in a variety of uniformly isotropic and liquid-like materials as two-dimensional still and moving images, just like ordinary optical microscopes.

First, UV-polymerized swollen nematic gels were prepared by mixing E44 with photo-polymerizable mesogen molecules and cross-linking agents and sealing them in a homogeneously oriented cell. We have succeeded in directly observing the "dynamic inhomogeneity" spontaneously generated during the cooling process of this swollen nematic polymer toward the glass transition temperature, as shown in Fig. 1. The image consists of 256x128 pixels, and the highest spatial resolution reaches about 0.4μm/pixel. The pseudo-color represents the relaxation time of orientation fluctuations, which is faster for colder colors and slower for warmer colors. Dynamic inhomogeneity images can also be recorded and analyzed as video recordings, and in this swollen nematic polymer, the dynamic inhomogeneity changes from time to time over a lifetime of a few seconds.

We observed three grades of sake produced in Kyoto and sold by the same brewery using a fluctuation microscope. Sake is nearly colorless and transparent, but it contains nano-scale alcohol clusters that repeatedly dissociate and aggregate. In the highest grade daiginjo, a complex tinted image is observed, indicating the presence of clusters of a wide variety of sizes. Dependent on the grade of sake, fluctuation microscope images indicate a decrease in the size of the alcohol clusters. It is obvious that it can be used not only to discriminate between different grades, but also in a variety of other situations, for example, in the manufacturing process, inspection of the occurrence of defective products, comparison of products produced in different years and so on.

Thus, the fluctuation microscope is a powerful new microscopic tool that can observe the dynamic space-time structure of any material system, including research, development, manufacturing, nature, and living organisms. For example, it can contribute to understanding the mechanisms of molecular clusters in mixed liquids, glass transitions, and sol-gel transitions. Alternatively, it can be used to observe optically transparent and liquid products such as alcoholic beverages, cosmetics, food products, and can be applied to product development, and inspection processes/degradation testing and recording. Thus, the fluctuation microscopic image provides a completely different information on the spatio-temporal structure in any kind of soft matter in comparison with conventional microscopes.

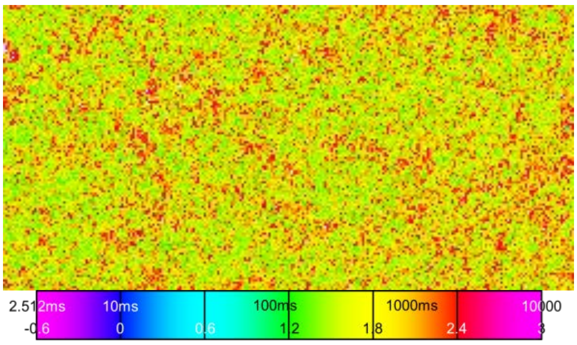

Fig.1 Fluctuation microscope image of the spontaneous dynamic heterogeneity in the LC-polymer (0.8μm/pixel, 200x100μm).

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1984/3 Bachelor of department of applied physics, The University of Tokyo

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1990/6 Ph. D (Engineering, The University of Tokyo)

1987/8 Assistant Professor, Department of Applied Physics, The University of Tokyo

1991/6 Assistant Professor, Institute of Industrial Science, The University of Tokyo

1999/10 Groupe Leader, ERATO Yokoyama Project, JST

2004/10 Researcher, Department of Nanotechnology, AIST

2005/8 Professor, Department of Physics, Graduate School of Science, Kyoto University

・**Main Publications**

1. S. Samitsu, Y. Takanishi, J. Yamamoto, Molecular manipulator driven by spatial variation of liquid-crystalline order, Nature Materials, 9, 816 - 820 (2010).
2. J. Yamamoto, I. Nishiyama, M. Inoue, H. Yokoyama, Optical isotropy and iridescence in a smectic 'blue phase', Nature, 437, 525 - 528 (2005).
3. J. Yamamoto, H. Tanaka, Transparent nematic phase in a liquid-crystal-based microemulsion, Nature, 409, 321 – 325, (2001).

Squeeze and Nanomechanics of Adsorbed Boundary Layers in a Lubricated Interface

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In order to simulate the squeeze of a confined thin film between two adsorbed layers on antagonistic solid surfaces, a numerical model was developed based on continuum mechanics using the generalized œdometric Reynolds equations extended to the case of heterogeneous films such as two adsorbed layers separated by a fluid film. This model accounted for the film compressibility and the substrate deformation for a sphere/plane configuration in both static and dynamic situations, under small-amplitude oscillations as used in non-contact dynamic surface forces or AFM measurements for instance.
After a short description of the numerical resolution method, the validation of the model was confirmed by confronting numerical results to theoretical and experimental ones. Our model was able to predict such as contact stress or complex stiffness as well as to provide physical insights of the squeeze mechanisms. The application of our numerical modeling to experimental squeeze of low viscosity fluid between fatty acid monolayers and polymer brush layers allowed one to assess the mechanical properties of the adsorbed boundary layers and to discuss the molecular organization within the squeezed interface.
This method opens new perspectives for measuring viscoelastic properties of adsorbed layers and their evolution under confinement.

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Biography:

Juliette Cayer-Barrioz graduated in Physics from the University of Grenoble in 1998 and in Mechanical Engineering from the Ecole Centrale de Lyon (ECL) in 2000 before obtaining her PhD in Materials Science from ECL in 2003 and her Habilitation in Mechanics in 2011. Since 2005, she has been associated with the CNRS. Her research activities at the Laboratoire de Tribologie et Dynamique des Systèmes (LTDS) in Ecole Centrale de Lyon focus on surface phenomena and dynamics of confined lubricated interfaces. Her multidisciplinary approach— based on unique experimental devices developed at the LTDS— combines physics, interfacial chemistry and mechanics, rheology and friction. After an 8-year contribution to the Laboratoire d'Excellence Manutech-Sise, she is now a member of the French National Committee of the CNRS in mechanics and one of the four editors of Tribology Letters. Her teaching activities at ECL, and beyond, address the physics and chemistry of interfaces and the rheology of complex media.

Main Publications

1. L. Frérot*, A. Crespo, J. A. El-Awady, M. O. Robbins, J. Cayer-Barrioz*, D. Mazuyer, *"From Molecular to Multi-Asperity Contacts: How Roughness Bridges the Friction Scale Gap"*, ACS Nano, 17, 2205–2211, 2023. doi:10.1021/acsnano.2c08435
2. D. Mazuyer, A. Ernesto, J. Cayer-Barrioz*, *"Theoretical modelling of film forming mechanisms under transient conditions: Application to deceleration and experimental validation"*, Tribology Letters, 65(1), 1-14 2017. doi: 10.1007/s11249-016-0801-9
3. N. Fernandez, R. Mani, D. Rinaldi, D. Kadau, M. Mosquet, H. Lombois-Burger, J. Cayer-Barrioz, HJ. Herrmann, ND. Spencer, L. Isa*, *"Microscopic mechanism for shear-thickening of*

non-Brownian suspensions", Phys. Rev. Lett. 111, 108301, 2013. doi:10.1103/PhysRevLett.111.108301

Abnormal Stribeck Curves of Concentrated Polymer Brushes in Macro and Nanoscales

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Concentrated polymer brushes (CPBs), significantly denser and thicker than conventional semi-dilute polymer brushes, show ultralow friction when swollen and lubricated by adequate liquid. Following the first attempt with atomic force microscopy found friction coefficient μ < 0.001 [1], CPBs have been improved for macroscale investigations, enabling recent attempts toward practical applications, such as wear mechanism investigation [2], durability improvement by surface texturing [3,4], and applications to seal technology [5,6] and to anti-icing technology [7]. This presentation discusses the fundamental lubrication property of CPBs: the abnormal Stribeck curves observed in macroscale experiments and nanoscale simulations (see **Figure 1**). The macroscale experiments used an ordinary pin/disc tribometer at Kyoto University, whereas the nanoscale simulations used the coarse-grained molecular dynamics (CGMD) method at Tohoku University. Their qualitatively similar results were quantitatively analyzed based on the Kelvin-Voigt viscoelastic foundation (KV-VEF) theory at Yokohama National University [8-10]. The dimensionless master curves of the KV-VEF theory enabled us to determine two viscoelastic parameters for each scale and clarify the mechanism of abnormal Stribeck curves shared beyond scales, even though units differed between experiments and simulations. A translation of CGMD to SI units found that the time constant of CPB in the macroscale was six orders of magnitude longer than in the nanoscale, probably caused by inhibiting solvent flow inside CPB due to different contact sizes.

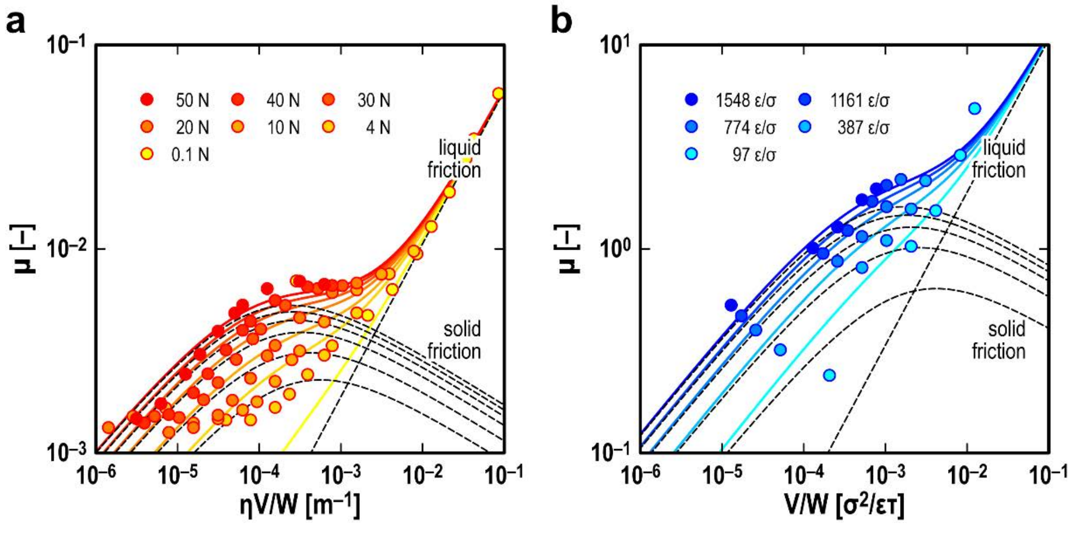

Figure 1. Abnormal Stribeck curves of CPBs branched for different contact loads, observed in (a) macroscale experiments and (b) nanoscale simulations; black straight line: liquid friction μ_{liquid} determined on the hydrodynamic lubrication theory; black curved line: solid friction μ_{solid} determined on the KV-VEF theory [8-10]; colored curved line: total friction $\mu = \mu_{liquid} + \mu_{solid}$.

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Major Fields: Tribology, Dynamics, Physics of Friction

Biography: Ken Nakano is a full professor at the Faculty of Environment and Information Sciences of Yokohama National University. He studied aeronautics and astronautics at the University of Tokyo and obtained his doctorate from the University of Tokyo in 1997. After working as an assistant professor at Saitama University from 1997 to 2000 and as an associate professor at Yokohama National University from 2000 to 2015, he obtained a full professorship at Yokohama National University in 2015. He specializes in the interdisciplinary field of tribology and dynamics, especially the physics of friction. He published over 100 reviewed papers. He received the Best Teacher Award from Yokohama National University in 2014, the Best Paper Award from the Japan Society of Mechanical Engineers in 2015, the Best Researcher Award from Yokohama National University in 2017, and the Best Paper Award from the Japanese Society of Tribologists in 2021. He was a board member of the Japanese Society of Tribologists from 2017 to 2019. Since 2024, he has been an Editor of Tribology Letters, published by Springer Nature.

Main Publications

1. C. Tadokoro, T. Nihira, K. Nakano, Minimization of friction at various speeds using autonomous viscosity control of nematic liquid crystal, *Tribol. Lett.*, **56**, 239-247 (2014).
2. T. Maruyama, K. Nakano, In situ quantification of oil film formation and breakdown in EHD contacts, *Tribol. Trans.*, **61**, 1057-1066 (2018).
3. K. Nakano, V. L. Popov, Dynamic stiction without static friction: The role of friction vector rotation, *Phys. Rev. E*, **102**, 063001 (2020).

In situ Analysis of a Rubber/Ice Interface

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According to U.S Department of transportation, 24 percent of car accident per year are due to the presence of snow/ice on roads. This includes small crashes and more severe accidents. In addition, according to the International Union for conservation of Nature, tires are the second source of microplastic pollution in oceans, reaching 28 percent in 2017.

In the context of improving icy road safety and reducing pollution, this work aims at analyzing and understanding the interfacial friction response of an ice-rubber contact, in a large range of environmental temperature, going down to -20°C, and of sliding velocity, ranging from 50µm/s to 1m/s. The material properties of the rubber samples provided by Michelin varied in terms of composition, of surface topography, of mechanical properties. The produced ice was homogenous and transparent, and it was subject to a controlled process of machining and thermalization. An *in-situ* contact area measurement methodology was developed during static loading and unloading and during sliding experiments. It allowed us to identify the relative influence of adhesion and viscoelastic contributions as a function of the temperature, as well as discuss the friction mechanisms in operando.

Investigating the viscoelastic properties of the rubber-ice interface using the low temperature surface force apparatus

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Ice friction plays a pivotal role in a variety of fields including transportation (*e.g.* black ice), winter sports (*e.g.* ice-skating) and machining (*e.g.* Arctic resource extraction). Each application utilises a variety of materials, such as synthetic rubbers and stainless steel, which possess differing properties, including viscoelasticity, surface roughness, and adhesion, all of which can influence friction. At the ice interface, a phenomenon called premelting is known, stemming from less interactions with neighbouring molecular species compared to those in the bulk. This leads to the formation of a premelted layer at the surface which possesses viscoelastic properties that are sensitive to the characteristics of the opposing sliding surface.

The resonance shear method, using the low temperature surface force apparatus, presents a novel approach to elucidating the viscoelastic behaviour of interfacial liquids [1]. The characteristics can be measured as a function of temperature, sliding velocity, and pressure at small junctions, typically of the order of ~10,000 μm^2, thereby bridging the gap between the nanoscopic and macroscopic. Here, we measure the viscoelastic response of a styrene-butadiene statistical copolymer at the ice interface as a function of temperature (*cf.* Figure 1) and styrene content (0, 5, 23, 45 and 100%). The rubber-ice interface showed a significant drop in viscosity relative to that of Si-Ice across a temperature range of -20 to -5˚C. Furthermore, it was observed that increasing styrene content increased the viscosity at temperatures below -10˚C, potentially attributable to the difference in elasticity of the copolymers. Finally, the viscous and elastic friction contributions were measured to understand how slipperiness at the ice interface is dependent on the material properties of the rubber (*cf.* Figure 2).

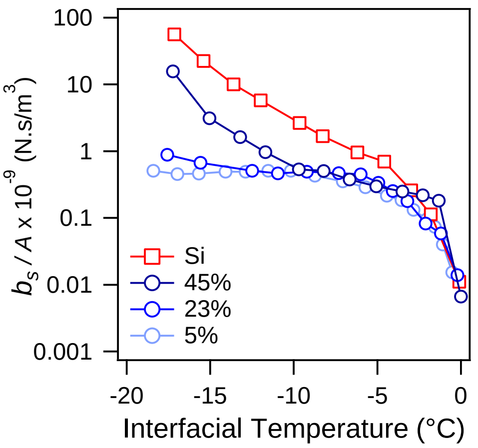

Figure 1. *Viscous parameter (b_s) normalised to area (A) as a function of temperature for the Si-Ice and Rubber-Ice interface.*

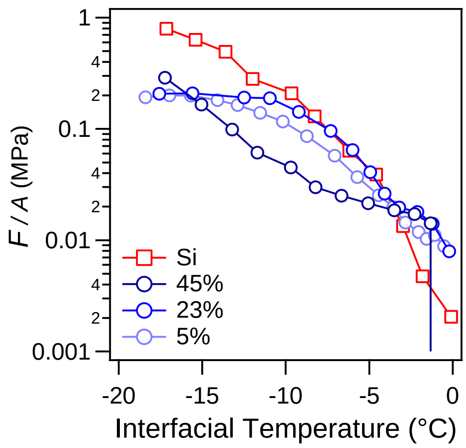

Figure 2. *Total friction (F) response at the Si-Ice and Rubber-Ice interface calculated from the viscous and elastic friction contributions (F_b and F_k respectively).*

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Major Fields: Soft Matter, Surface Forces and Tribology

Biography:

2024	Postdoctoral Research Associate, Kurihara Laboratory (Tohoku University)
2023	Postdoctoral Research Assistant, Briscoe Group (University of Bristol)
2018-2023	PhD (Physical and Theoretical Chemistry), *Surface forces and boundary lubrication by novel amphiphilic block copolymers in nonpolar media*, Briscoe Group (University of Bristol)
2016-2017	Industrial Placement, Printed Electronics Formulations, Dycotec Materials Ltd, UK
2014-2018	MSci Chemistry with Industrial Experience (University of Bristol)

<u>Awards</u>

2021	XRR Synchrotron proposal, Diamond Light Source, I07 (3 days, SI26893)
2021	SANS proposal, ILL, D33 (5 days, 9-10-1639)
2020	SANS proposal, ISIS, SANS2D (3 days, RB2010516)
2019	M4 Colloids Conference Best Poster Prize

Main Publications

1. **M. C. Stevens**, Nicholas M. Taylor, Xueying Guo, Hadeel Hussain, Najet Mahmoudi, Beatrice N. Cattoz, Alice H.M. Leung, Peter J. Dowding, Brian Vincent, Wuge H. Briscoe*, Diblock bottlebrush polymer in a non-polar medium: Self-assembly, surface forces, and superlubricity, *Journal of Colloid and Interface Science*, 2024, **658**, 639-647
2. L. Matthews, **M. C. Stevens**, R. Schweins, P. Bartlett, A. J . Johnson, R. Sochon, W. H. Briscoe*, Unexpected observation of an intermediate hexagonal phase upon fluid-to-gel transition: SDS self-assembly in glycerol, *Colloid and Interface Science Communications*, 2021, **40**, 100342

Effect of Hyperbranched Polymers as Additive on Lubrication Properties of Base Oil

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A Polymers have been used as additives of lubricants. The polymers used in the previous studies have been limited to those of linear chain structures. In general, the use of low viscosity lubricants is effective in the hydrodynamic lubrication (in high shear rate and low load conditions) but increase in the friction and wear in boundary lubrication (in low shear rate and high load conditions). In order to resolve this issue, we studied the lubrication properties of hyperbranched polymers as additives in a base oil (PAO).

The viscosity values of the hyperbranched (A) and linear (B) polymer solutions (5 mg/mL) in PAO were measured at 40 °C using an ultra-trace viscometer. The viscosity of the polymer A was 16.0 mPa·s and slightly increased compared the value of PAO (13.7 mPa·s). Polymer B exhibited more increase in the viscosity (17.7 mPa·s).

Fig. 1(a) and **(b)** show the resonance curves measured for the solutions of polymer A and B between the mica surfaces at various loads (*L*), respectively. In order to compare the friction of different polymer systems, the peak intensity (U_{out}/U_{in}) was normalized by the amplitude of the solid contact (SC, no sliding) peak. The intensity ratio to the SC peak at L = 4.0 mN was found to be polymer A (12%) < polymer B (20%) < PAO (35%), indicating that polymer A has low friction and higher lubricity.

In order to confirm the good correlation between the nanoscopic and macroscopic lubrication properties of the polymer solutions in PAO, friction tests were performed on the linear and hyperbranched polymer solutions as well as PAO alone (without polymer additives). **Fig. 2** shows plots of friction coefficients for PAO alone, PAO with the polymer A, and with the polymer B as a function of (velocity, *V*)/(load, *L*) at 40 °C (Stribeck curves). In the boundary lubrication (V/L < 0.05), the addition of polymer A significantly reduced the coefficient of friction. The good lubricity of polymers was demonstrated in both of the nanoscopic and macroscopic scale. The hyperbranched polymer would be a lubricant additive that can achieve both lower viscosity and lower friction in the boundary lubrication.

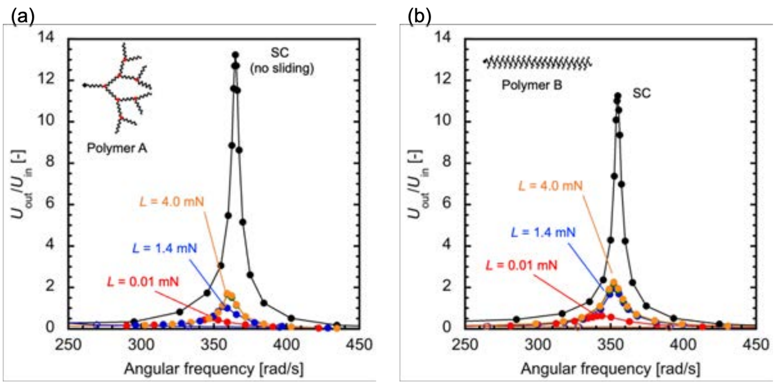

Fig. 1 Resonance curves for the solutions of (a) hyperbranched polymer A and (b) linear polymer B in PAO at various loads (*L*).

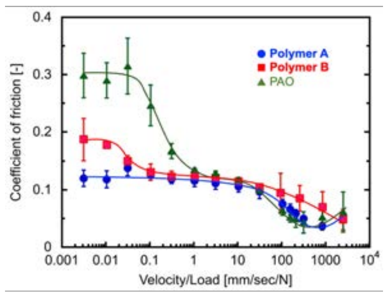

Fig. 2 Friction coefficients of lubricants as a function of velocity/load. The solid lines are included to guide the eye.

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Major Fields: Interfacial chemistry, Surfactant chemistry

Biography:

Work

2018–present	Assistant Professor, NICHe, Tohoku University
2013–2018	Assistant Professor, Department of Industrial Chemistry, Faculty of Engineering, Tokyo University of Science

Education

2013	Ph.D. in Engineering, Tokyo University of Science

Main Publications

1. Takahashi, Y.; Mizukami, M.; Tsujii, Y.; Kurihara, K. "Surface Forces Characterization of Concentrated PMMA Brush Layers under Applied Load and Shear" *Langmuir*, **40**(1), 325-334 (2024)
2. Takahashi, Y.; Koizumi, N.; Kondo, Y. "Active Demulsification of Photoresponsive Emulsions Using Cationic–Anionic Surfactant Mixtures" *Langmuir*, **32**(3), 683-688 (2016)
3. Takahashi, Y.; Yamamoto, Y.; Hata, S.; Kondo, Y. "Unusual viscoelasticity behaviour in aqueous solutions containing a photoresponsive amphiphile" *J. Colloid Interface Sci.*, **407**, 370-374 (2013)

Evolution of stress/displacement fields and contact area of PDMS sphere during oblique loading and shearing

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Under increasing shear, the contact between a rough elastomer and a rigid surface, for example in the case of contact between a tire and a road surface, may undergo significant changes in terms of morphology of the micro-contacts due to the presence of wear [1]. In such contacts, it is also possible to observe strong variation of the local pressure during shearing that may be related to the wear patterns that are frequently observed in literature [2]. Such morphological and loading changes are indeed expected to affect all macroscopic responses of the interface. In particular the transition to full sliding may differ significantly from the classical behavior described by Cattaneo and Mindlin [3].

In this study, our aim is to analyze the contact stress/displacement state during oblique loading and shearing of a sphere made of model elastomers representative for tire tread materials. These analyses are performed by measuring not only the classical evolution of macroscopic normal and tangential forces but also that of the true contact area and interfacial stress/displacement fields.

The experimental tests consist in using a complex loading representative of the behavior of a tire during rolling. To do so, we perform a single normal loading/unloading cycle during a continuous shearing motion representative of one tire revolution in a new generation opto-mechanical device recently developed in our laboratory [4]. The latter enables rich contact loading through five simultaneous and independent degrees of freedom with simultaneous high-resolution monitoring of all three forces and three moments at the contact interface. It also enables high-resolution in-situ visualization of the contact area, giving access to in-operando, measurements in the real contact area of the stress/displacement fields through advanced image analysis techniques [5].

This experimental procedure makes it possible to study the effect of several characteristic parameters, such as the ratio between “landing” and sliding speed or the maximal normal force. Prior to using complex charged rubber, we performed preliminary tests on unworn spheres of uncharged elastomer (PDMS) seeded with markers to monitor the evolution of contact area and interfacial displacement field via image analysis. Characterizing this complex kinematic should help us understanding the initiation of wear phenomenon in the contact area. Subsequent tests on tire-type rubber will enable us to extend our comprehension to more realistic rubber materials.

<u>References</u>

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2. Huang , …, L., Loubet, J-L., Sotta, P., A new test method to simulate low-severity wear conditions experienced by rubber tire materials, Wear 410-411, 72--82 (2018)

3. K. L. Johnson, Contact Mechanics, Cambridge University Press, 1985

4. M. Guibert, C. Oliver, T. Durand, T. Le Mogne, A. Le Bot, D. Dalmas, J. Scheibert, and J. Fontaine, A versatile flexure-based six-axis force/torque sensor and its application to tribology, Review of Scientific Instruments 92, 085002 (2021)
5. J. Lengiewicz, …, C. Courbon, D. Dalmas, J. Scheibert, J. Mech. Phys. Solids 143, 104056 (2020)

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Major Fields: Contact mechanics, Rubber, Materials mechanics

Biography:

Education:

- **Engineer INSA de Rouen** (National Institute of Applied Sciences) school of engineering
- **Master's degree** in Design Engineering and materials mechanics (INSA de Rouen)
- Internship (4 months) at ETH Zurich/NCCR Digital Fabrication laboratories
  - Additive Manufacturing: developing a digital fabrication method to build with concrete

Professional experiences:

- **PhD at CNRS, LTDS, Ecole Centrale de Lyon** (France) 2nd year
  - Abrasion wear of elastomers : relationship with the local stress/strain state at the contact interface
  - Study of the evolution of a « tyre/road » type contact during representative loading cycles
- **Engineer at Laboratoire de Physique, ENS de Lyon**, ANR Paraperf (JO Paris 2024)
  - Development of a power meter for athletic wheelchair, managing a research project
  - Participating to several research projects (sport sciences, drafting in cycling)
- Internship and Engineer (10 months) at Comtoyou Racing (Belgium)
  - Data engineering in a European and World Touring Car Racing team: optimising drivers cars' performances, contributing to race wins and championship titles

Interfacial Friction in Carbon Nanotubes (CNTs)/Ceramics Composites: A ReaxFF Study to Reveal CNT Reinforcing Mechanisms

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SiC ceramics materials play an important role as structural materials in the industries of aerospace, automotive, and power plants, because of their extraordinary strength and high hardness. However, from the perspective of safe utilization, it is vital to enhance the naturally low fracture toughness of ceramics materials. To improve the fracture toughness, it is suggested to add carbon nanotubes (CNTs) into ceramics matrix as the reinforcing agents. However, the CNT reinforcing results studied previously are still controversial, in lack of the optimized composite design. Unlike conventional reinforcing agents, such as solid fibers, CNTs are composed of multi-layered tube structures, making the conventional composite designing theory not suitable for them. When adding CNTs into ceramics, the frictional dynamics among CNT layers, as well as the interaction between CNTs and ceramics (CNT/ceramics friction) occur at atomic scale, remaining unclear. Hereby, the purpose of this study is to clarify the CNT reinforcing mechanisms considering atomic-scale interfacial frictions within the CNT/ceramics composites [1]. In this study, the effect of interlayer friction and CNT/ceramics friction on the mechanical properties of CNT/ceramics composites are studied by reactive molecular dynamics (MD) methods. Here, reactive force field is adapted to MD simulations to calculate the generation and dissociation of bonds for the discussion of interfacial behaviors. SiC is applied as ceramics for its wide application.

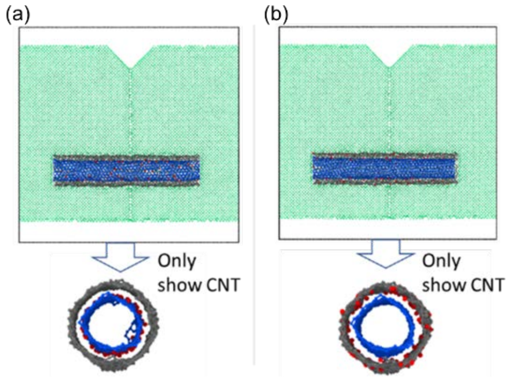

Fig. 1. Si doped CNT/SiC models with doping on (a) inner and (b) outer CNT.

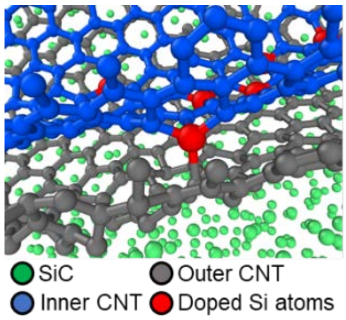

Fig. 2. Interwall crosslinking.

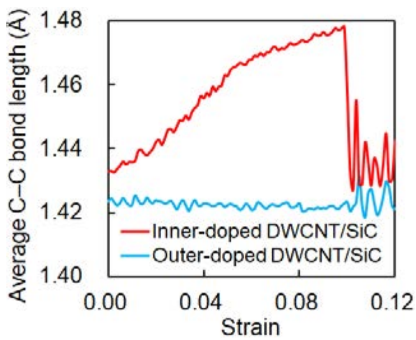

Fig. 3. The average C–C bond length of the inner CNT as a function of strain.

For the purpose of studying the effect of interlayer friction on CNT reinforcement, we design introducing crosslinking among CNT layers to generate varying levels of interlayer friction. Si doping, as a common chemical modification method to control crosslinking [2], is applied to the outer and inner layers (Fig. 1) of double-walled CNTs (DWCNTs). As a result, Si doping on the inner CNT (inner-doped DWCNT) generates interwall crosslinking, indicating enhanced interwall interaction (Fig. 2). Meanwhile, interwall crosslinking does not occur in the outer-doped DWCNT/SiC composites. To assess the effectiveness of CNT reinforcement through doping, we investigated the mechanical properties. Our results show that doping Si atoms on the inner CNT leads to an approximate 3% improvement in Young's modulus and a 1% increase in toughness. In contrast, doping on the outer CNT results in a modest 0.3% increase in Young's modulus, but an 8% decrease in toughness. The mechanical properties of the composites indicate that inner-doped DWCNTs provide greater reinforcement than outer-doped DWCNTs. To investigate the underlying mechanism, we analyze the evolution of the average C–C bond length of the inner CNT during tensile simulations (Fig. 3), and observe significant stretching of the inner CNT in the inner-doped DWCNT/SiC composites, while no such stretching occurs in the outer-doped DWCNT/SiC composites. Overall, it is found out that the interwall crosslinking and improved interwall interaction cause the inner CNT to stretch, resulting in better reinforcement by inner-doped DWCNT than outer-doped DWCNT.

Next, we aim to investigate the effect of the interaction between CNTs and SiC (CNT/SiC interfacial friction) on the mechanical properties of composites. Experimental studies have shown that annealing can induce structural changes at the CNT/matrix interfaces in composite [3, 4]. However, the mechanism of interface structural changes affecting mechanical properties of CNT/ceramics composite is unrevealed. Therefore, we aim to control the annealing temperatures of composites to produce varying levels of CNT/SiC interfacial friction, allowing for the quantification of annealing's effect on interfacial friction and mechanical properties. CNT/amorphous SiC composites are constructed and annealed at temperatures ranging from 700 to 2300 K. Tensile simulations are performed afterwards at 300 K to observe the effect of annealing. As shown in Fig. 4, the mechanical properties including Young's moduli and tensile strength, show a volcano-type dependence on annealing temperatures. At the temperature range of 300~1700 K, mechanical properties increase with annealing temperatures. This enhancement is attributed to stronger CNT/SiC interfacial interactions, which lead to greater degree of CNT stretching and better reinforcement. Meanwhile, at the temperature of 1700~2300 K, mechanical properties decrease with increasing annealing temperatures. This is because that CNT structures get more crashed inside the composites as the annealing temperature rises, resulting in poorer reinforcement. Hereby, the best result is at the temperature range of 1400~1900 K. It is shown that the best improvement on CNT reinforcement comes from a good balance of strong CNT/SiC interface and CNT structure intactness.

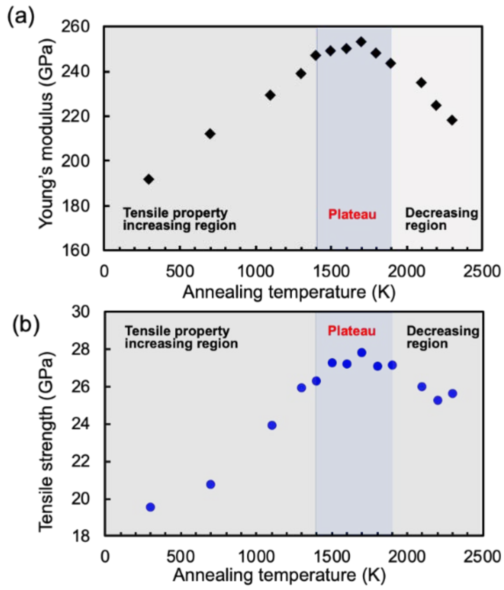

Fig. 4. Mechanical properties of CNT/SiC composites annealed at different temperatures: (a) Young's moduli and (b) tensile strengths.

The details will be discussed during presentation.

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Dr. Yixin Su is an Assistant Professor in Computational Materials Science at Tohoku University, specializing in fuel cells, catalysts, and composite materials. She earned her Ph.D. in Engineering in 2023 and has published in leading journals, including *ACS Applied Nano Materials*. In recognition of her academic excellence, Dr. Su received the prestigious *SCCJ-SUYAMA Fellowship* from the Society of Computer Chemistry in 2019. She has been invited to present her research at high-profile conferences, including the International Conference and Expo on Advanced Ceramics and Composites (ICACC) 2023 in the U.S. and the International Symposium celebrating the 80th Anniversary of the Tohoku Branch of the Chemical Society of Japan. Fluent in English, Japanese, and Chinese, Dr. Su fosters global collaborations and brings a unique, interdisciplinary perspective to computational materials science challenges.

Main Publications
1. Y. Su, J. Zhang, Q. Chen, Y. Wang, N. Miyazaki, Y. Ootani, N. Ozawa, M. Kubo, J. Comput. Chem. Jpn 18 (2019) 259262.
2. Y. Wang, Y. Su, J. Zhang, Q. Chen, J. Xu, S. Bai, Y. Ootani, N. Ozawa, M.I. de Barros Bouchet, J.M. Martin, K. Adachi, M. Kubo, ACS Appl. Nano Mater. 3 (2020) 72977304.
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In-layer inhomogeneity of molecular dynamics in quasi-liquid layers of ice

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Quasi-liquid layers (QLLs) are present on the surface of ice and play a significant role in its distinctive chemical and physical properties. These layers exhibit considerable heterogeneity across different scales ranging from nanometers to millimeters. Although the formation of partially ice-like structures has been proposed, the molecular-level understanding of this heterogeneity remains unclear. Here, we examined the heterogeneity of molecular dynamics on QLLs based on molecular dynamics simulations and machine learning analysis of the simulation data [1]. We demonstrated that the molecular dynamics of QLLs do not comprise a mixture of solid- and liquid water molecules. Rather, molecules having similar behaviors form dynamical domains that are associated with the dynamical heterogeneity of supercooled water. Nonetheless, molecules in the domains frequently switch their dynamical state. Furthermore, while there is no observable characteristic domain size, the long-range ordering strongly depends on the temperature and crystal face. Instead of a mixture of static solid- and liquid-like regions, our results indicate the presence of heterogeneous molecular dynamics in QLLs, which offers molecular-level insights into the surface properties of ice.

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1. Ikki Yasuda, Katsuhiro Endo, Noriyoshi Arai and Kenji Yasuoka, “In-layer inhomogeneity of molecular dynamics in quasi-liquid layers of ice”, Commun. Chem., 7, 117 (2024).

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Biography:

I am currently Ph.D. student at Keio University under the supervision of Professor Yasuoka. As a DC1 Research Fellow from the Japan Society for the Promotion of Science, my doctoral research is centered on the prediction of phase separation in intrinsically disordered proteins. I obtained my bachelor's degree in mechanical engineering in 2021, followed by a master's degree in computational mechanics in 2023. During my previous research, I focused on the application of machine learning to analyze molecular dynamics simulation data. Furthermore, from 2023 to 2024, I am undertaking a Guest Ph.D. position at the University of Copenhagen, conducting research within Professor Kresten Lindorff-Larsen's group on coarse-grained molecular models of RNA.

Main Publications

1. Ikki Yasuda, Katsuhiro Endo, Eiji Yamamoto, Yoshinori Hirano, and Kenji Yasuoka, "Differences in ligand-induced protein dynamics extracted from an unsupervised deep learning approach correlate with protein–ligand binding affinities" Commun. Biol., 5, 481 (2022).
2. Ikki Yasuda, Yusei Kobayashi, Katsuhiro Endo, Yoshihiro Hayakawa, Kazuhiko Fujiwara, Kuniaki Yajima, Noriyoshi Arai, and Kenji Yasuoka, "Combining molecular dynamics and machine learning to analyze shear thinning for alkane and globular lubricants in low shear regime", ACS Appl. Mater. Interfaces, 5, 8567–8578 (2023).
3. Ikki Yasuda, Katsuhiro Endo, Noriyoshi Arai and Kenji Yasuoka, “In-layer inhomogeneity of molecular dynamics in quasi-liquid layers of ice”, Commun. Chem., 7, 117 (2024).

Molecular Simulation of Friction Phenomena at the Ice-Polymer Interface

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Despite the sub-freezing temperatures, the ice surface melts, forming a pseudo-liquid layer, designated the premelting layer. This layer forms not only at the ice-vapor interface but also at the ice-polymer (rubber) interface, thereby exerting a considerable influence on the characteristics of the ice surface. While the behavior of the premelting layer at the ice-vapor interface has been extensively investigated, the behavior of this layer at the ice-polymer interface remains unclear. A comprehensive understanding of the behavior of the premelting layer at the ice-polymer interface is of paramount importance for the development of innovative applications such as winter tires for automobiles. Nevertheless, the behavior of this layer under frictional conditions remains challenging to elucidate due to the influence of various factors, including temperature, pressure, speed, and rubber surface roughness.

In this study, the TIP-4P/ICE model was employed to analyze the density distribution. Prior experimental studies have demonstrated that the melting behavior of the premelting layer varies depending on the type of polymer, including polystyrene and polyethylene oxide[1]. In molecular simulations, the equilibrium structures of PS, PVA and PEO were generated, and the melting behavior at the ice-polymer interface was analyzed at various temperatures using density distribution and other parameters. Figure 1 shows the structure of each polymer, the system diagram, and the density distribution for each polymer.

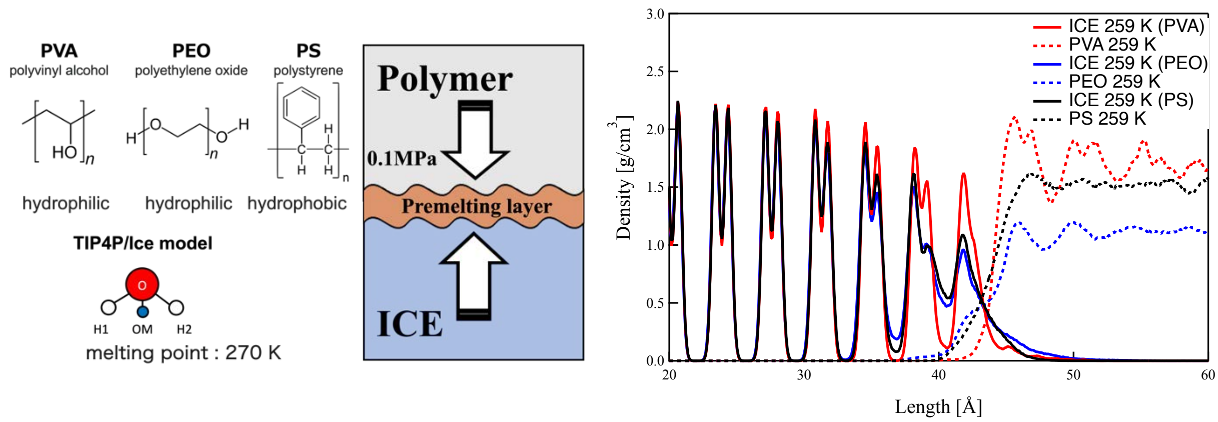

Figure 1. Density distribution at the ice-polymer interface.

First, the effect of polymer type on the ice-polymer interface was investigated: the degree of ice melting varied with polymer even at 259 K, with the first peak of the ice density distribution being the lowest for PEO. In the case of PEO, the penetration of water molecules into the interior of the polymer was observed, suggesting that the hydrophilic nature of PEO promotes the formation of a hydration layer with water molecules and the melting on the ice surface.

Next, friction at the ice-polymer interface was simulated. The system is divided as shown in Figure 2, and shear simulation is performed by applying acceleration to the top of the polymer. Figure 2 shows the temperature of each layer when the system is divided by 2 nm in the Y direction. The temperature increased at the top of the polymer under acceleration and 259 K at the bottom of the ice under temperature control. The interface temperature changed with friction velocity. Figure 3 shows the change in friction velocity and interface temperature.

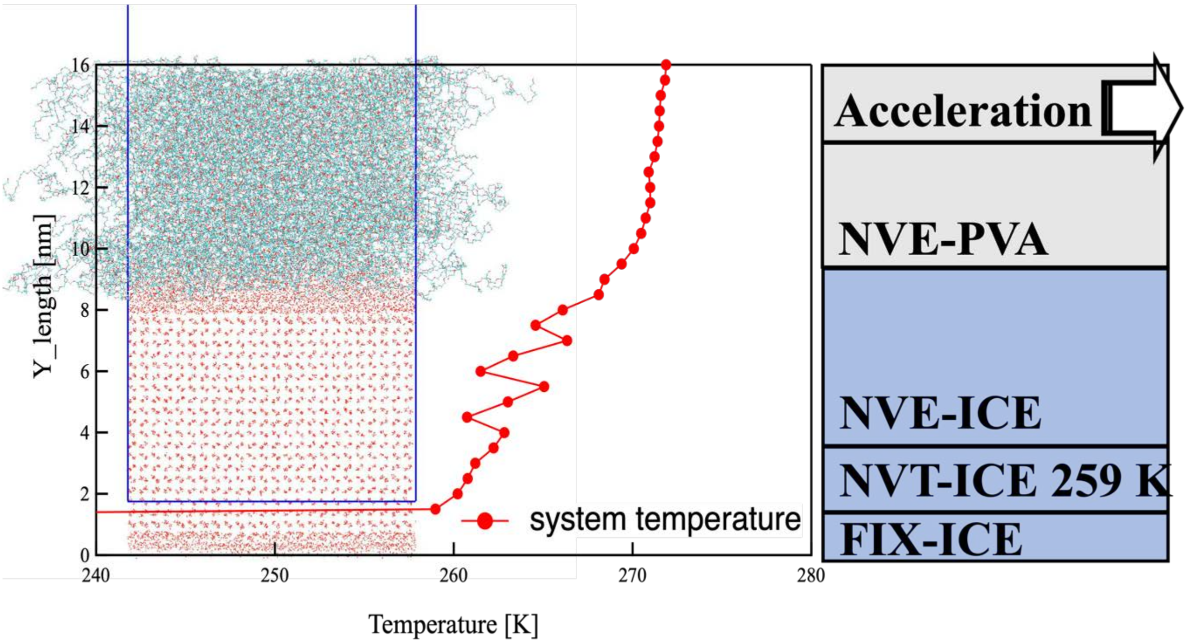

Figure 2. System temperature in friction simulation

By controlling the acceleration, the friction velocity was varied from 0.04 to 0.9 nm/s. Currently, the temperature variation at each velocity is being compared with experimental data to elucidate the phenomenon.

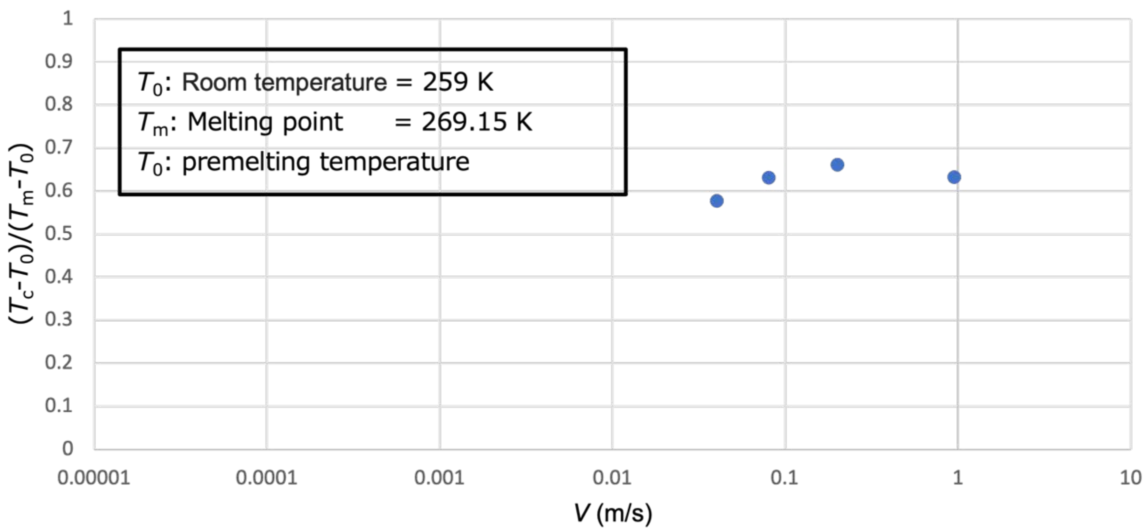

Figure 3. Variation of ice-polymer interface temperature with sliding velocity

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09/2020 – 03/2022	Master of Science in Open Environment Science, Graduate School of Science and Technology, Keio University, Japan (Completed)
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Main Publications

1. T. Sato, Y. Kobayashi, T. Michioka, and N. Arai: "Self-Assembly of Polymer-Tethered Nanoparticles with Uniform and Janus Surfaces in Nanotubes", Soft Matter, Vol. 17, pp. 4047-4058, (2021).
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3. T. Sato, K. Esashika, E. Yamamoto, T. Saiki, and N. Arai: "Theoretical Design of a Janus-Nanoparticle-Based Sandwich Assay for Nucleic Acids", International Journal of Molecular Sciences, Vol. 23, pp. 8807, No. 15, (2022).

Fracture and Degradation Mechanisms in Nitrided Steel Surface through Reactive Molecular Dynamics Simulations

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The surface hardness of metallic materials is a crucial factor that influences their resistance to wear and fatigue. Nitriding treatment is widely applied to steel to enhance its surface hardness by forming an outermost compound layer and subsurface diffusion zone. The compound layer is hard and composed of polycrystals of Fe_3N and Fe_4N. However, under certain treatment conditions, voids may form within this layer. The voids near the surface have been noted to decrease the surface hardness and may act as initiation sites for cracks during tensile deformation[1]. This study aims to investigate the effect of these voids on the tensile deformation behavior of nitrided steel. Reactive molecular dynamics simulations were conducted to analyze the deformation behavior of Fe_4N polycrystalline models, both with and without voids. The simulation models used in this study are illustrated in Figure 1. Figure 1(a) shows the model with voids, while Figure 1(b) visualizes the voids in the model. We also constructed a comparative model without voids. Tensile simulations were performed by applying a strain rate of 20 ns^{-1} in the *x*-direction. ReaxFF was employed to describe the interatomic interactions[2]. We have developed ReaxFF parameters for Fe and N systems that can reproduce the lattice constant and Young's modulus of Fe_4N and Fe_3N with the Jax-reaxff framework[3]. The simulation results revealed that, in the void-free model, a phase transformation from FCC to HCP occurred before any intergranular cracking. In contrast, in the model with voids, the coalescence of multiple voids caused cracks to form at the grain boundaries (Figure 2). In this model, almost no phase transformation was observed. These results show that voids have a significant effect on the durability and mechanical performance of nitrided steel under tensile stress. On the day of the presentation, we will also discuss the degradation mechanisms in corrosive environments.

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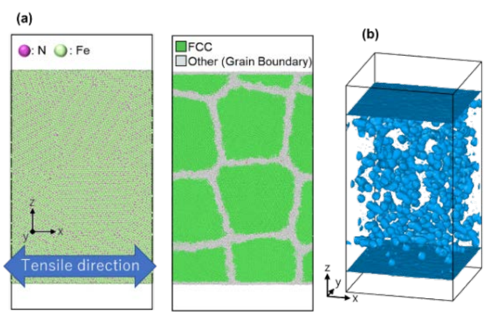

Fig. 1 (a) Fe_4N with voids model. The right image shows the morphology of the crystal structure with FCC-structured Fe atoms in green and grain boundary atoms in white. (b) Only the voids and the model surface are shown in blue For the model in (a).

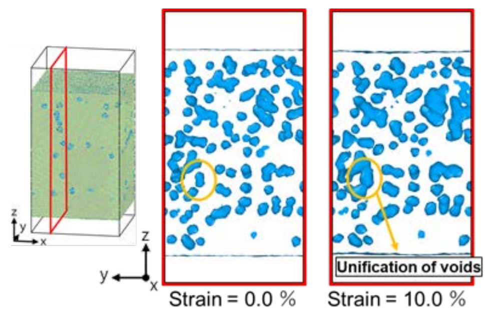

Fig. 2 Snapshots of the voids within the red-framed area of the voids model in the MD simulation. The left image shows the initial state, and the right image shows the state under strain of 10.0 %.

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Major Fields:
Molecular dynamics simulation, Metallic materials, Wear, Deformation process

Biography:
Mizuho Yokoi is taking a doctoral course in material science at Tohoku University. Her research interest is the corrosive wear mechanisms of metallic materials using molecular dynamics simulations, and she has been actively conducting research in this field for the past two years. She is selected as a Japan Society for the Promotion of Science (JSPS) Research Fellowship for Young Scientists.

Main Publications
1. Yokoi, M., Kawaura, M., Asano, Y., Chen, Q., Ootani, Y., Ozawa, N. & Kubo, M. Effect of water and oxygen at sliding interface on friction and wear of diamond-like carbon/steel: Reactive molecular dynamics simulations. *J. Comput. Chem. Jpn. -int,* 8, 2022-0009 (2022). https://doi.org/10.2477/jccjie.2022-0009
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Friday 15th of November 2024

Confined Liquids Studied by Resonance Shear Measurement：
Molecular Mechanism of Lubrication

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Lubricant oils are used in many mechanical systems to reduce the friction and wear. A major and simple approach for reducing friction is to decrease the viscosity of lubricant oils, which directly reduces the friction in the hydrodynamic regime. There is, however, a drawback in this approach. The low viscosity lubricant often causes high friction and wear in the boundary lubrication regime, where the velocity is slow and/or the applied load is high. This behavior in the boundary lubrication regime has been interpreted, as in Borden-Tabor model, due to the contact of rough surfaces of moving parts after lubricant molecules are removed from the gap between them.

We may ask whether there is no lubricant molecules remain in the gap, and if they could exist what their properties and relation with macroscopic friction are. Our recent researches employing resonance shear measurement (RSM) have revealed a new view of the boundary lubrication regime that some lubricant molecules remain in a nano-space between solid surfaces, and their effective viscosity increase in one to several orders of magnitudes,[1-3] as commonly seen for confined liquids, which usually exhibit different properties from those of the bulk state due to restriction of their molecular packing and motions and their interaction with substrate surfaces.[4]

This paper reviews researches employing RSM on confined liquids (interfacial water, ionic liquid and lubricant oils). First, differences in properties of interfacial water due to hydration of alkali ions[5] and to hydrogen bonding[6] are discussed in terms of the distance range of hydration, and their properties. Second, ionic liquids bearing the same cation (1-butyl-3-methylimidazolium, [C_4mim]) and different anions (bis(trifluoromethanesulfonyl)amide, [NTf_2]; tetrafluoroborate, [BF_4]) form different ion packing at the interface, which determines lubrication properties of ionic liquids.[7] Their different interfacial structures are indicated by the molecular simulation and confirmed by the X-ray diffraction.[8] A novel feature of boundary lubrication is presented based on properties of confined lubricants, which will promote developing new lubricants to reduce energy consumption due to friction. These approaches will broaden the potential of molecular design for future lubricants.[1-3]

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Major Fields: Colloid and Interface Science, Surface Forces Measurement

Biography:

Kazue Kurihara is a Research Professor of Tohoku University at the New Industry Creation Hatchery Center (NICHe) and holds the title of Professor Emeritus. She has been a faculty member at the Institute of Multidisciplinary Research for Advanced Materials since 1997. Her research focuses on the measurement of surface forces in materials science, through which she aspires to establish a new field she refers to as 'forcemetry.' She has developed innovative instruments and methods, such as a twin-path surface forces apparatus (SFA) for opaque samples, which not only broadens the range of materials that SFA can analyze, but also allows simultaneous electrochemical and fluorescence measurements. Her resonance shear measurement method provides a highly sensitive technique for monitoring lateral forces, such as friction.

Her studies include the characterization of solid-liquid interfaces, liquids confined between solid surfaces, polymer brushes, and gels. She has also made significant contributions to the development of new instrumentation for these characterizations. Recently, her research group has been actively engaged in X-ray diffraction studies of liquids confined in nanometer spaces between solid surfaces and in the study of ice surfaces using a low-temperature SFA.

Main Publications

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Multiscale analysis of the tribological behavior of polymer-based composite in contact with steel under grease lubrication: from nanoscale tribofilms to macroscale damage

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Polyamide 66 is widely used for sliding parts, in many applications such as resin worm gear. Glass or carbon fibers are usually added to increase its strength. Grease may be used to improve the tribological behavior of the contact.

In this study, the tribological behavior of glass or carbon fiber reinforced-polyamide 66 composite in contact with carbon steel under high contact pressure, sliding, and grease lubricated conditions is studied. Measurement of mechanical properties and SEM observations of composite sliding surfaces after different sliding cycle numbers indicate that sliding induces characteristic damage of the surface (peeled off fibers and scratching of polyamide) and a degradation in mechanical properties. These lead to an increase in friction and creep of the composite. The damage to the composite surface and the increase in contact temperature due to sliding have great effects on the tribological properties, compared to the presence of wear debris in grease and wear on the steel. The effects of different parameters (hardness of the steel, temperature…) on the tribological properties are investigated. The tribochemical reactions related to zinc carboxylate additives in grease are studied through XPS and ToF-SIMS analyses which revealed the formation of a carboxylate tribofilm on the steel surface and a zinc sulfide reactive film on the PA66 surface.

Tribological multiscale analysis is performed, by looking at nanoscale tribofilms formed on the rubbing surfaces and by considering the effect of the microstructure of the material (size, shape and amount of fibers) on the macroscale damage of the two contacting bodies.

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Major Fields: Tribology, wear of materials

Biography:

1999: diploma of engineer and master at Ecole Centrale de Lyon

2002: PhD in tribology at Ecole Centrale de Lyon

Since 2003: Ass. Prof. at Ecole Centrale de Lyon; research activities at LTDS on tribology and wear of materials

Since 2022: coordinator of the International Research Network (IRN) between CNRS, INSA de Lyon, Ecole Centrale de Lyon and Tohoku University

Main Publications

1. T. ZURCHER, G. BOUVARD, J.-Ch. ABRY, E. CHARKALUK, V. FRIDRICI, **Effect of the scanning strategy and tribological conditions on the wear resistance of IN718 obtained by Laser Metal Deposition**, *Wear* (534–535), article 205152, 19 pages, 2023. https://doi.org/10.1016/j.wear.2023.205152.
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Molecular simulation and machine learning for friction mechanism

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Molecular dynamics (MD) simulation is a powerful computational method to calculate physical properties and analyze molecular mechanisms for various molecules. We perform the MD simulations for multiple systems to clarify the friction mechanism. However, the high computational costs of large-scale and long-time MD simulations limit the method's applicability. In addition, the analysis of molecular mechanisms is typically complex due to the complexity of molecular behavior. To address these general problems of MD simulations, we proposed two novel machine learning methods focusing on (1) the acceleration of time evolution in MD simulations and (2) the detection of representative molecular behavior that characterizes systems. For the first one, we proposed the machine learning method based on generative adversarial nets (GANs) to accelerate time evolution in MD simulations. This method obtains the efficient time evolution method from the short-term MD data to generate long-term dynamical statistics. For the second one, we applied deep neural networks to calculate statistical distances between different ensembles and detect representative molecular behavior in systems.

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Main Publications

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In situ X-ray computed tomography study of a sphere/plane contact under normal and shear loadings

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Nowadays, to study in-situ or in operando the contact and friction behavior of an interface, measurements are mostly made through optical devices which requires the use of at least one optically transparent material and limit the analysis to only the evolution of the interface and more specially to the real contact area [1]. Thus information outside this confined zone are most of time inaccessible. In this study, we overcame these two limits by using an X-ray Computed Tomography (XRCT). Starting from the very few pioneering studies [2], we adopted a more model approach to investigate by XRCT the classical laws of contact mechanics in a model sphere on plane contact. Our main objective was to examine the relationship between loading conditions, material properties, contact area and bulk deformation in 3D.

Thanks to an experimental loading device installed in a laboratory tomograph [3], we were able to obtain 3D images of a contact between a smooth PDMS sphere against a smooth PMMA plane for different loading conditions: pure normal loading/unloading (indentation) and shear loading under constant normal force (friction test). First, after segmentation of the 3D volumes, we extracted the evolution of real contact area and the surface displacement field of the PDMS specimen as function of the loading conditions (for indentation and friction tests) [4]. We then compared these evolutions to established experimental results and to the classical theoretical models of contact mechanics [5]. Finally, we performed Digital Volume Correlation analysis by analyzing the displacement of dispersed particles that were inserted inside the PDMS sphere. We, thus, measured the 3D bulk displacement, strain and stress fields and compared them again with the prediction of theoretical models [4].

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Main Publications

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3. J. Lengiewicz, M. de Souza, M. Lahmar, C. Courbon, D. Dalmas, et al.. Finite deformations govern the anisotropic shear-induced area reduction of soft elastic contacts. Journal of the Mechanics and Physics of Solids, Elsevier, 143, pp.104056. ⟨10.1016/j.jmps.2020.104056⟩. ⟨hal-02562750v2⟩ (2020)

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1. Dancette, S.; Fabrègue, D.; Massardier, V.; Merlin, J.; Dupuy, T.; Bouzekri, M. Experimental and Modeling Investigation of the Failure Resistance of Advanced High Strength Steels Spot Welds. Engineering Fracture Mechanics 2011, 78 (10), 2259–2272. https://doi.org/10.1016/j.engfracmech.2011.04.013.
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Main Publications in Tribology

1. Effect of ion beam-sputtered silica films on the wear behavior of ion-implanted silicon nitride
   DOI: 10.1016/j.surfcoat.2004.09.021
2. Nano-structure and tribological properties of B+ and Ti+ co-implanted silicon nitride
   DOI: 10.1016/j.nimb.2004.09.011
3. Improvement in wear resistance of high-strength and high-toughness silicon nitride modified by ion implantation
   DOI: 10.1111/j.1551-2916.2004.01167.x
4. Investigation of wear surfaces in Si+-implanted uni-directionally aligned silicon nitride using TEM and XPS
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5. Surface analytical studies of ion-implanted uni-directionally aligned silicon nitride for tribological applications
   DOI: 10.1016/j.nimb.2003.09.024
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   DOI: 10.1016/S0955-2219(03)00243-7