



# STLE Tribology Frontiers Conference

**2020 STLE Tribology Frontiers Conference**  
Co-sponsored by the ASME Tribology Division

November 9-13, 2020

**Program Guide**  
as of November 9, 2020

2020 STLE Virtual Tribology Frontiers Conference  
November 9-13, 2020

Preliminary Program-at-a-Glance  
As of 11-6-20 – Subject to Change

**Monday, November 9, 2020**

**Networking – 8:30 – 9:00am**

**Welcome and Introductions – 9:00 – 9:15 am**

**Keynote Session –9:15 – 9:55 am**

**Keynote Presentation:**

Ali Erdemir, Texas A&M University: *Frontiers of Catalyst-driven Tribochemistry: Implications for Friction and Wear*

**Technical Sessions – 10 – 11 am**

1A – Energy, Environment and Manufacturing I  
1B – Fluid Lubrication I  
1C – Surfaces & Interfaces I

**Meet the Experts – 11 – 11:30 am**

**Keynote Edition** – Ali Erdemir, Texas A&M University

**Industry Edition** - *Emerging Modelling Techniques and AI in Tribology* with Prathima Nalam, SUNY University at Buffalo and Sarah Blanck, Centre de Recherche Total de Solaize

**Technical Sessions – 11:30 am – 12:30 pm**

1A – Energy, Environment and Manufacturing I  
1B – Fluid Lubrication I  
1C – Surfaces & Interfaces I

**STLE Connect-(Exhibits & Posters) – 12:30 – 1 pm**

**Keynote Session –1 – 1:55 pm**

**Keynote Presentation:**

Carmel Majidi, Carnegie Mellon University: *Challenges at the Interface in Soft, Stretchable Electronics*

**Technical Sessions – 2 – 3:20 pm**

2A – Energy, Environment and Manufacturing II  
2B – Fluid Lubrication II  
2C – Surfaces & Interfaces II

**Meet the Experts – 3:20 – 4 pm**

**Keynote Edition** - Carmel Majidi, Carnegie Mellon University

**Industry Edition** - *Next Generation Lubricants and Bearings*, Michael Kotzalas, The Timken Company

**Tuesday, November 10, 2020**

**Networking – 8:30 – 9:00am**

**Keynote Session –9:00 – 9:55 am**

**Keynote Presentation:**

Rosa Espinosa-Marzal, University of Illinois at Urbana-Champaign: *Modulating Slip, Adhesion and Friction of Graphene Via Substrate-Induced Doping*

**Technical Sessions – 10 – 11:00 am**

3A – Tribochemistry I  
3B – Surfaces & Interfaces III  
3C – Lubricants I

**Meet the Experts – 11 – 11:30 am**

**Keynote Edition** - Rosa Espinosa-Marzal, University of Illinois at Urbana-Champaign

**Industry Edition** - *Soft Matter Tribology* with Nicholas Spencer and Angela Pitenis, University of California-Santa Barbara

**Technical Sessions – 11:30 am – 12:30 pm**

3A – Tribochemistry I  
3B – Surfaces & Interfaces III  
3C – Lubricants I

**STLE Connect-(Exhibits & Posters) – 12:30 – 1 pm**

**Keynote Session –1 – 1:55 pm**

**Keynote Presentation:**

Jean-Francois Molinari, EPFL, Switzerland: *Revisiting Archard's Wear Model: A Dialog Between Scales*

**Technical Sessions – 2 – 3:20 pm**

4A - Tribochemistry II  
4B – Surfaces & Interfaces IV  
4C – Lubricants II

**Meet the Experts – 3:20 – 4 pm**

**Keynote Edition** - Jean-Francois Molinari, EPFL  
**Industry Edition** - 2D and Carbon-based Materials with Diana Berman, University of North Texas

**Wednesday, November 11, 2020**

**Networking – 8:30 – 9:00am**

**ASME Workshop – 9:00 am – 12 pm**  
**(Separate Registration Required)**

**Technical Sessions - 8:00 – 10 am**

5A – Materials Tribology I  
5B – Surfaces & Interfaces V  
5C – Tribochemistry III

**Break – 10 – 10:20am**

**Technical Sessions – 10:20 am – 12 pm**

5A – Materials Tribology I  
5B – Surfaces & Interfaces V

**STLE Connect-(Exhibits & Posters) – 12:00 – 1 pm**

**6A - Special Plenary Symposium – Beyond the Cutting Edge: Highlights from Tribology Letters – 1 pm – 4:00 pm**

**Thursday, November 12, 2020**

**Networking – 8:30 – 9:00am**

**Keynote Session –9:00 – 9:55 am**

**Keynote Presentation:**

Patricia Iglesias Victoria, Rochester Institute of Technology, New York: *Protic Ionic Liquids: Economical and Low-Toxicity Lubricants and Additives*

**Technical Sessions – 10 – 11 am**

7A – Materials Tribology II  
7B – Lubricants III  
7C – Machine Elements & Systems I

**Meet the Experts – 11 – 11:30 am**

**Keynote Edition** - Patricia Iglesias Victoria, Rochester Institute of Technology, New York  
**Industry Edition** - *Emerging Experimental Techniques* with Tevis Jacobs, University of Pittsburgh and Kerry Cogen, Infineum USA L.P.

**Technical Sessions – 11:30 am – 12:30 pm**

7A – Materials Tribology II  
7B – Lubricants III  
7C – Machine Elements & Systems I

**STLE Connect-(Exhibits & Posters) – 12:30 – 1 pm**

**Keynote Session –1 – 1:55 pm**

**Keynote Presentation:**

David Burris, PhD, University of Delaware: *Cartilage Tribology and the Biomechanics of Joint Health*

**Technical Sessions – 2 – 3:20 pm**

8A – Materials Tribology III  
8B – Lubricants IV  
8C – Machine Elements & Systems II

**Meet the Experts – 3:20 – 4 pm**

**Keynote Edition** - David Burris, PhD, University of Delaware  
**Industry Edition** - *Ionic Liquids* with Filippo Mangolini, The University of Texas at Austin and Shouhei Kawada, Miyatake Laboratory

**Friday, November 13, 2020**

**Networking – 8:30 – 9:00am**

**Keynote Session –9:00 – 9:55 am**

**Keynote Presentation:**

Izabela Szlufarska, PhD, University of Wisconsin-Madison: *Microstructural and Chemical Evolution of Frictional Contacts*

**Technical Sessions – 10 – 11 am**

9A – Biotribology I  
9B – Lubricants V

**Meet the Experts – 11 – 11:30 am**

**Keynote Edition** - Izabela Szlufarska, PhD, University of Wisconsin-Madison  
**Industry Edition** - *Tribochemistry and Film Formation* with Manel Rodriguez Ripoll, AC2T research GmbH and James Ewen, Imperial College of London

**Technical Sessions – 11:30 am – 12:30 pm**

9A – Biotribology I  
9B – Lubricants V

**STLE Connect-(Exhibits & Posters) – 12:30 – 12:45 pm**

**Closing Comments: 12:45 – 1:00 pm**

**Keynote Session –1 – 2:00 pm**

**Keynote Presentation:**

John A. Rogers, Northwestern University: *Electronic and Microfluids Systems That Softly Interface to the Skin*

**Closing Celebration – 2 - 2:20 pm**

Monday, November 9, 2020

**9 – 9:15 am - Welcome and Introductions**

**9:15 – 9:55 am - Keynote Session**

Ali Erdemir, Texas A&M University

*Frontiers of Catalyst-Driven Tribochemistry: Implications for Friction and Wear*

1A

Virtual Breakout Room 1

**Energy, Environment and Manufacturing I**

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**Session Chair:** Nicolas Demas, Argonne National Laboratory, Lemont, IL

**10 - 10:20 am**

**3436061: Design of SiO<sub>2</sub> Nanoparticle Deposited 3D Connected Porous Aluminum Alloy Electrode Surfaces for Rechargeable Batteries**

Swarn Jha, Siddhi Mehta, Yan Chen, Alaa Elwany, Hong Liang, Texas A&M University, College Station, TX

Open-pored hierarchical structured surfaces for electrodes have great promise in improving the performance of rechargeable batteries. However, the manufacturing of such nano- and micro-structured electrode surfaces have been expensive, inefficient, time-consuming, and commercially unfeasible. In this research, we used additive manufacturing to surface engineer a highly organized, open pore, 3D interconnected surface of AlSi<sub>12</sub> alloy deposited with SiO<sub>2</sub> nanoparticles. High-resolution synchrotron micro-tomography was employed to observe fine morphological details. Electrochemical experiments were done to study the effects of the structure of the materials as potential electrodes for lithium-ion batteries. We found that the ion transport and the kinetic diffusion, between the active material and the electrolyte, are mainly dependent on the size, geometry, and distribution of the pores present on the electrodes. The design, manufacturing procedures, and resulting electrodes are valuable in developing new rechargeable batteries in the future.

**10:20 - 10:40 am – Open Slot**

**10:40 - 11 am**

**3439422: Thermal Management in Battery Electric Vehicle (BEV)**

Harsha Nanjundaswamy, Dean Tomazic, Joel Deussen, Madhura Medikeri, Chen Duan, Andreas Mayer, FEV North America Inc., Auburn Hills, MI

In this presentation, an insight into EDU and battery thermal management techniques and challenges will be described in greater detail. Furthermore, an in-depth review of the advanced direct cooling techniques of EDU and Battery will be outlined. Additionally the advancements in integrated power electronics and high voltage conductors and the associated thermal management techniques will be presented. Towards the conclusion, the presentation will outline the future trends in EDU, power electronics and battery technology and how the thermal management is becoming a critical step in system design and optimization.

**11 - 11:30 am - Meet the Experts**

**11:30 - 11:50 am**

**3439455: Influence of Fluids on the Operational Efficiency of Transmissions and Drivetrain Components**

Kiran Govindswamy, Dean Tomazic, Tom D'Anna, Thomas Wellmann, FEV North America Inc., Auburn Hills, MI

The use of innovative drivetrain technologies including conventional and electrified propulsion systems is expected to play an increasingly important role in helping OEMs meet fleet CO<sub>2</sub> reduction targets for 2025 and beyond. This presentation will showcase a systematic process aimed at understanding the overall energy flow in a vehicle over the course of a representative fuel economy drive cycle. Examples from testing of a hybrid vehicle will be utilized to describe the losses in various portions of the drivetrain. The influence of various sub-systems on the transmission efficiency will be highlighted. The importance of transmission fluids on the efficiency of both conventional and electrified drivetrains will be discussed. Industry trends aimed at minimizing the losses related to hydraulics and drivetrain fluids will be shared and aspects of improved hydraulics and low-viscosity fluids will be illustrated using examples from case studies on transmissions and drivetrain components.

**11:50 am - 12:10 pm**

**3413729: Latest in Biosynthetic Base Oils – Evaluating Estolide Performance Characteristics in Expanding Viscosity Ranges**

Mark Miller, Debby Neubauer, Biosynthetic Technologies, Indianapolis, IN

Estolides are an environmentally acceptable base oil that is referred to as a “biosynthetic”. They are known for their performance characteristics and use as a petroleum replacement in lubricant formulations. The number of estolide products being offered to the market is growing as new viscosities are being offered. We look at how these products compare to each other and to other commercial base oils in the industry. Estolides are very versatile and can be used in several industries and products within the marine, automotive, and industrial markets. Findings from example formulations will show performance benefits of these estolides.

**12:10 pm - 12:30 pm - Open Slot**

**1B**

Virtual Breakout Room 2

**Fluid Lubrication I**

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**Session Chair:** Rob Dwyer-Joyce, University of Sheffield, Sheffield, South Yorkshire, United Kingdom

**Session Vice Chair:** Amir Kadiric, Imperial College London, London, United Kingdom

**10 - 10:20 am**

**3420426: Elasto-HydroDynamic Lubrication with Mixture in Point Contact**

Fan Zhang, Université de Lyon, INSA Lyon, CNRS, LaMCoS, Lyon, France

Classical Elasto-HydroDynamic lubrication theory assumes that a single piezo-viscous fluid lubricates rolling contacts. In reality, lubrication systems often involve fluids other than neat lubricants. Depending on different applications, the lubricating fluid could be a mixture of lubricant and environmental fluid. Two types of mixture in EHD lubricated point contact are investigated in this study. The first one is the water in oil mixture, where water droplets are suspended in oil as emulsion[1]–[4]. The second one is oil mixed with refrigerant; the latter is volatile and miscible with the former in refrigeration compressor application[5], [6]. Depending on the applications, the key questions are different. In the first case (emulsion), we will address the problem of modeling water entrance into the contact and its effect on film thickness. In the second case, the main question is the possible evaporation of part of the mixture at the exit of the contact.

**10:20 - 10:40 am**

**3432447: Piston Ring on Liner Lubrication Monitoring in a Marine Diesel Engine Using Ultrasound**

Jack Rooke, Xiangwei Li, Rob Dwyer-Joyce, University of Sheffield, Sheffield, South Yorkshire, United Kingdom, Henry Brunskill, Peak to Peak, Sheffield, United Kingdom, Mattias Stark, Winterthur Gas & Diesel Ltd, Winterthur, Switzerland

Marine diesel engines are designed based around high thermal efficiency, high fuel economy and durable performance although this leads to substantial emissions levels. One route to cut emissions is to reduce frictional losses, granting a higher operational efficiency. The interaction with the greatest frictional impact is the piston ring on cylinder liner contact. Traditional measurements on liners required highly invasive instrumentation often requiring transducers to be mounted on the internal surface of the liner whereas with ultrasound, this oil film can be studied by instrumenting piezoelectric transducers to the outer surface of the liner. Through the variation in ultrasonic pulses detected by these transducers at a range of engine speeds and oil feed rate, parameters such as oil film thickness and ring scuffing can be quantified non-invasively. Optimisation of factors such as oil film thickness has the potential for significant reductions in emissions, wear and oil consumption.

**10:40 - 11 am**

**3439445: Numerical and Experimental Investigation of Aerostatic Bearing with Applications to High-Frequency Rotation (More Than 100 kHz)**

Rajdeep Deb, Beat Meier, Solid State Nuclear Magnetic Resonance, ETH Zurich, Zurich, Switzerland, Dirk Wilhelm, Institute of Applied Mathematics and Physics, ZHAW, Winterthur, Switzerland, Patrick Jenny, Institute of Fluid Dynamics, ETH Zurich, Zurich, Switzerland

Sample rotation around an axis inclined by about  $54^\circ$  with respect to the magnetic field (the "magic angle") is used in solid-state nuclear magnetic resonance spectroscopy to obtain high spectral resolution which is the key to determine molecular structure and dynamic, e.g. in biomolecules or battery materials. The rotation frequencies required exceed 100 kHz and operation in a strong magnetic field (20 Tesla) is required. The aerostatic bearing used for such rotors limit the spinning stability under fast spinning conditions. We describe the optimization of the bearing design for such systems based on a modified Reynolds equation applicable to small bearing size. A stability analysis was performed to predict a suitable bearing design and the results are compared with experimental data for different bearing configurations.

**11 - 11:30 am - Meet The Experts**

**11:30 - 11:50 am**

**3410408: Visualization of Micro Cavity Flow of Surface Textured Mechanical Seal by Particle Tracking Velocimetry**

Iwa Ou, Shogo Fukuda, Eagle Industry Co., Ltd., Sakado-shi, Saitama-Ken, Japan

We have realized mechanical seals with both low friction and superior sealing capabilities by surface texturing technology [1-2]. Rayleigh step is a typical texturing pattern which combine shallow grooves with deep grooves. The shallow grooves generate dynamic pressure and are designed by in house hydrodynamic lubrication calculation. The measured thickness of thin liquid film is successfully reproduced by it [1]. On the other hand, the deep grooves leads fluid to the shallow grooves efficiently but are difficult to design since the turbulence flow in micro cavity have to be solved computationally. In addition, the flow are also difficult to measure directly in high velocity and small visualization area. Particle Tracking Velocimetry was utilized to measure the flow in deep grooves with different shapes. The measured particle flow is also compared to that calculated by commercial CFD software (Ansys Fluent). Details of experimental setup and how PTV can help the design of surface texturing systematically will be presented.

**11:50 am - 12:10 pm - Open Slot**

12:10 pm - 12:30 pm - Open Slot

1C

Virtual Breakout Room 3

## Surfaces & Interfaces I

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**Session Chair:** Robert Fleming, Arkansas State University, Jonesboro, AR

**Session Vice Chair:** Adriana Quacquarelli, INSA Lyon, Villeurbanne, France

**10 - 10:20 am**

### **3419267: A Multi-Scale Strategy for Wear Modeling of Diamond Tools**

Adriana Quacquarelli, INSA Lyon, Villeurbanne, France

A granular material consisting in a mixture of debris and a liquid (i.e. a slurry) can be treated as an equivalent fluid with well-defined rheological properties and it is able to shear under a confined pressure and an imposed shear rate between two material surfaces. If the granular flow is abrasive for the contact surfaces, the wear can be discretized as the sum of wear contribution own to each grain. We study the effect of the flow in terms of hydrodynamic pressure generated between the two surfaces [1] and wear effects on the surfaces themselves [2]. A wear equation is written as a function of debris properties and micromechanical properties of the surface.

We apply the model considering, as a particular case of study, the wear of DIT (Diamond Impregnated Tools) caused by the abrasive flow generated during the cutting process [3]. The validation is made comparing the numerical results with the experimental ones.

**10:20 - 10:40 am**

### **3419310: Third-Body Flow Regime Influence on the Surface Response to Tribological Loading**

Olivier Bouillanne, Guilhem Mollon, Aurélien Saulot, Sylvie Descartes, INSA de Lyon, Villeurbanne, France, Nathalie Serres, Guillaume Chassaing, Karim Demmou, Safran Aircraft Engines, Moissy-Cramayel, France

In aircraft turbofans, blades and central disk are attached with a dovetail joint. In this mechanical contact, particles of third-body are created, flow inside the contact, and damage first bodies surfaces. The rheology of the third-body flow can show various regimes: laminar, turbulent, pasty, agglomerated, etc. [2].

The software MELODY is used to model this flow, and provides some understanding on how third body properties (stiffness, cohesion and viscosity) modify the tribological loading on first bodies. We especially focus our study on stress tensor variations in space and time, and investigate how to apply constitutive damage models (such as the triaxiality approach) to relate these variations to surface evolutions and eventually to wear.

**10:40 - 11 am**

### **3420027: Improving the Frictional Performance of Elasto-Hydrodynamic Lubricated Contacts by Applying Fast Laser Surface Texturing of Spherical Samples**

Guido Boidi, AC2T research, Wiener Neustadt, Austria, Philipp Grützmaier, Carsten Gachot, TU Wien, Vienna, Austria, Amir Kadiric, Daniele Dini, Imperial College London, London, United Kingdom, Izabel Machado, Francisco J. Profito, Polytechnic School, University of São Paulo – USP, São Paulo, Brazil

Textured surfaces generally improve tribological performances, however the texturing manufacturing techniques require additional operations and costs, being often not economically feasible for real

engineering applications. This experimental study aims at applying fast laser texturing technique on curved surfaces for obtaining superior tribological performances with reduced manufacturing time. Femtosecond pulse laser (Ti-Sapphire) and Direct Laser Interference Patterning (Nd:YAG) were used for manufacturing dimple and groove patterns on curved steel surfaces (ball samples). Tribological tests were performed under elasto-hydrodynamic lubricated contact varying sliding-rolling conditions using ball-on-disk configuration. Furthermore, a specific interferometry technique for rough surfaces was used to measure film thickness of smooth and textured surfaces. Smooth steel samples were used as reference bench material. The results showed that dimples promoted friction reduction (up to 20%) compared to reference smooth surfaces, whereas grooves generally brought drawbacks. In addition, dimples promoted full film conditions at lower speeds, even occupying less textured area compared to the other textures. Fast texturing techniques could potentially be used for improving the tribological performance in engineering applications.

## **11 - 11:30 am - Meet The Experts**

**11:30 - 11:50 am**

### **3420313: Molecular Dynamics Simulations of Dislocation Confinement Effects in Core-Shell Nanostructures**

Robert Fleming, Arkansas State University, Jonesboro, AR

Recently, a novel nanostructured surface composed of patterned arrays of Al/a-Si core-shell nanostructures (CSNs) has been shown to have a desirable combination of ultra-low friction (COF  $\sim 0.015$  against a diamond counter face) and high durability. When subjected to instrumented nanoindentation, the individual CSNs show an unusual mechanical response characterized by almost complete deformation recovery, even beyond the elastic limit. Fundamentally, this mechanical behavior is hypothesized to be a result of a back-stress that develops in the confined Al core during compression loading that causes nucleated dislocations to retrace their paths or otherwise annihilate during unloading. In this study, molecular dynamics simulations are utilized to investigate the role that geometry and material properties play on the unique mechanical behavior of CSNs, with special attention paid to the core-shell interface structure, the core size/shape, and supporting stress calculations. Knowledge of the physical mechanisms that contribute to the deformation-resistant properties of Al/a-Si CSNs will potentially allow for control of dislocation dynamics in confined volumes and will further enable the development of novel material systems.

**11:50 am - 12:10 pm**

### **3480741: Ab Initio Insights into the Interaction Mechanisms between Boron, Nitrogen and Oxygen Doped Diamond Surfaces and Water Molecules**

Carlos Ayestaran Latorre, Imperial College London, London, United Kingdom

Diamond and diamond-like carbon coatings are used in many applications ranging from biomedicine to tribology. Several dopants have been tested to modify the hydrophilicity of these surfaces, since this is central to their biocompatibility and tribological performance in aqueous environments. Despite the large number of experimental investigations, an atomistic understanding of the effects of different dopants on carbon film hydrophilicity is still lacking. In this study, we employ ab initio calculations to elucidate the effects of B, N, and O dopants in several mechanisms that could modify interactions with water molecules. These include the adsorption of intact water molecules on the surfaces, minimum energy pathways for water dissociation, and subsequent interactions of hydrogenated and hydroxylated surfaces with water molecules. We find that the dopants considered enhance hydrophilicity, but they do so through different means. Most notably, B dopants can spontaneously chemisorb intact water molecules and increase interactions in H-bond networks.

## **12:30 – 1 pm - STLE Connect (Exhibits & Posters)**

**1 – 1:55pm - Keynote Session**

Carmel Majidi, Carnegie Mellon University

### ***Challenges at the Interface in Soft, Stretchable Electronics***



**Energy, Environment & Manufacturing II**

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**Session Chair:** Benjamin Gould, Argonne National Laboratory, Chicago, IL

**2 - 2:40 pm****3439417: "SPOTLIGHT" - Study of Vibration Wear in Plug-In Hybrid Vehicle Engine**

Weizi Li, Shell (Shanghai) Technology Limited., Shanghai, China, Yunfei Wang, Qin hao Fan, Zhi Wang, Tsinghua University, Beijing, China, Taylor Robert, Shell Global Solutions UK, London, United Kingdom

At times plug-in hybrid vehicle (PHEV) is powered only by electricity, hence engine does not operate and is not lubricated well, subsequently is under severer stress of vibration on road. Thus, this study initiated by Shell and Tsinghua University is aimed to identify possible lubrication challenge in such case. As first step, vibration data acquisition from a PHEV is done through dynamometer and real driving, amplitude and frequency characteristics of engine vibration are analyzed. Next, in order to simulate extreme conditions in pure electricity mode, the PHEV engine is installed on a specifically designed rig to produce accelerated aging resulting from vibration. Lastly, engine is teared down for measurement and rating. The test results suggest fretting wear can be intensified in PHEV as we find corrosion-like wear pattern on the journal bearing close to fly wheel and scratches which indicated abrasive wear on con-rod bearings.

**2:40 - 3 pm****3452741: Optimization of Tribological Parameters of 4340 Steel Machining Processes with the Use of Laser Surface Texturing**

Demófilo Cortés, Mónica Herrera-Maldonado, Gabriela Trouselles, Rodrigo Montalvo, Universidad de Monterrey, San Pedro Garza Garc, NL, Mexico, Laura Pena-Paras, Martha Rodríguez, University of Monterrey, San Pedro, Nuevo Leon, Mexico

Machining processes are one of the most widely used and indispensable manufacturing processes. The nature of such a process is high in friction between the workpiece and cutting tools, so the inserts have a short life, the finished parts are of low quality, and a lot of energy is consumed. The first part of the research consisted of the optimization of cutting parameters and concentration of nanoparticles in the cutting fluid to increase the useful life of cutting tools, decrease in roughness workpiece surface area and energy consumption savings of a 4340 steel machining process. This process was carried out on a computerized numerical control machining machine and three levels were defined to vary the different cutting parameters and the amount of nano particles. Finally the optimized values of the input parameters were obtained to obtain the best results in the output values. For the second part of the project the optimized parameters were used and a laser texturing pattern was added to the inserts as another variable to observe the behavior of the process, determine if there is an effect in improving the output variables and establish which of the patterns used works best for minimizing roughness, power consumption and wear. After 18 runs, benefits were obtained in the surface finish of the machined part of up to 37%, decreases in the tool radius of up to 10.4% and reductions in energy consumption of up to 5.4%

**3 - 3:20 pm - Open Slot****3:20 - 4 pm - Meet The Experts****Fluid Lubrication II**

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**Session Chair:** Rosa Espinosa-Marzal, University of Illinois Champaign-Urbana, Urbana, IL  
**Session Vice Chair:** Michael Kotzalas, The Timken Company, North Canton, OH

**2 - 2:20 pm**

**3409433: Lubricity and Viscosity of N-Butanol and Its Mixtures in Ultra-Low-Sulfur Diesel**

Gustavo Molina, John Morrison, Cesar Carapia, Valentin Soloiu, Georgia Southern University, Statesboro, GA

Tribological effects of mixing N-Butanol in ultra-low-sulfur diesel (ULSD) fuel, which led to an increase in lubricity of the mixtures, were assessed by tribometer-wear and viscometry. A unique change in viscosity caused by mixing N-Butanol with ULSD fuel also was found. The viscosity of the diesel decreases when mixed with the N-Butanol, and this change in viscosity could cause increased wear rates and changes in the friction force. But while the viscosity of the mixture is lower than those of the diesel and N-Butanol alone, the viscosity vs temperature curve for heated mixtures shows an inflexion to higher viscosities for higher temperature, and larger than those of N-Butanol at same temperatures. Also the addition of about 25% N-Butanol yields a lower tribometer-wear-value as compared to those of pure N-Butanol and ULSD. Results are presented on the viscosity and tribometer-tested wear and lubricity of N-Butanol and of its mixtures in ULSD diesel, and future research plans are outlined.

**2:20 - 2:40 pm**

**3439323: Correlating Adsorption Behavior and Tribological Performance of Organic Friction Modifiers**

Sendhil Poornachary, Febin Cyriac, Pui Shan Chow, A\*STAR Institute of Chemical and Engineering Sciences, Singapore, Singapore, Naoki Yamashita, Tomoko Hirayama, Kyoto University, Kyoto, Japan

Understanding the adsorption mechanism of organic friction modifiers (OFMs) on metal surfaces, in relation to their friction reducing abilities, can aid design of novel lubricant additives to improve fuel efficiency in automotive engines. In principle, the functional mechanism of OFM involves anchoring of its polar head group onto the metal surface, with the hydrocarbon tail oriented perpendicular to the surface; the adsorbed layers of OFM are difficult to compress under high loads but can be easily sheared at the hydrocarbon tail interfaces, thereby reducing friction in the boundary and mixed lubrication regimes. Notwithstanding this general mechanism, several structural factors influence the adsorption behavior and hence tribological performance of the OFM. Herein, we investigate the adsorption behavior of OFMs using two different experimental techniques. First, a quartz crystal microbalance with dissipation monitoring (QCM-D) is used to determine adsorption kinetics of OFMs containing different polar head groups but with a similar hydrocarbon tail structure. Among the additives, oleyl amine interacts strongly with the metal surface leading to thicker film formation. This observation is consistent with the frictional response of these additives measured using a Mini Traction Machine. Second, neutron scattering experiments are performed to determine the thickness of OFM layers adsorbed at the metal/oil interface and gain insights into the structure of the lubrication layer.

**2:40 - 3 pm - Open Slot**

**3 - 3:20 pm - Open Slot**

**3:20 - 4 pm - Meet The Experts**

2C

Virtual Breakout Room 3

**Surfaces & Interfaces II**

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**Session Chair:** Luke Thimons, University of Pittsburgh, Pittsburgh, PA

**Session Vice Chair:** Zhe Chen, Pennsylvania State University, University Park, PA

**2 - 2:20 pm**

**3418264: The Generalized Reference Lever: A Simple, Reliable and Traceable Calibration Method for Arbitrary Normal and Friction Forces**

Arnab Bhattacharjee, David Burris, University of Delaware, Newark, DE

No reliable calibration method has yet been developed for scanning probe friction measurements. As a result, the tribology basic science literature sits on a foundation of uncalibrated measurements that may or may not be comparable across studies. This paper aims to resolve this critical problem. Essentially, we adapt a mature and widely accepted technology, the pre-calibrated reference lever, as a means to store forces from a traceable calibration standard of fixed range (e.g. microbalance) and scale them to accommodate the load ranges (normal and lateral) of an arbitrary scanning probe. This paper presents the theory, demonstrates a simple prototype device and method of use, and validates the approach along several independent lines of analysis. As the results demonstrate, the generalized reference lever method is simple, reliable, and traceable. The concept, approach, and validation will be especially easy to grasp and implement by those who are practiced with the reference lever method of normal force calibration.

**2:20 - 2:40 pm**

**3435077: Investigating the Effect of Nanoscale Roughness on Macroscale Adhesion in Hard Contacts: Experimental Measurements of Ruby on Polycrystal Diamond**

Luke Thimons, Abhijeet Gujrati, Tevis Jacobs, University of Pittsburgh, Pittsburgh, PA, Antoine Sanner, Lars Pastewka, University of Freiburg, Freiburg, Germany

Adhesion in hard-material contacts is highly sensitive to roughness. However, still lacking is a quantitative, experimentally validated framework to describe this dependence. In this investigation, adhesion tests were performed between macroscale ruby spheres and four polycrystalline diamond materials of varying roughness. The topography of the spheres and substrates were characterized across length scales from millimeters to nanometers. Thousands of adhesion tests per material demonstrated broad distributions of pull-off forces, with systematic variations between materials. The topography-dependent adhesion was analyzed assuming an exponential form of the adhesive interaction potential. Scientifically, this analysis demonstrated that the range of adhesive interaction between the materials extends out to several nanometers. Practically, this analysis suggested how multi-scale roughness can be used to understand and predict roughness-dependent adhesion.

**2:40 - 3 pm**

**3435749: Capturing Fretting Fatigue with FEA Framework**

Iyabo Lawal, Matthew Brake, Rice University, Houston, TX

FEA models that include frictional response of the contact patch, can provide insights about the fretting fatigue phenomena observed in metal samples subjected to high cycling at low slip amplitudes. Friction models that can capture the stick-slip and hysteresis of the interface are needed. This work seeks to see how interface response to frictional loading. Simulation results of surface and subsurface stress will be compared with fretting experiments that includes surface characterization with Confocal Microscope and SEM. Using ANSI 304 SS substrates, displacement-based models and velocity-based friction models will be compared and used to simulate local material deformation in response to prescribed loading conditions. Results of this study can provide a tool to evaluate interface response and can provide insights about how to design interface geometries and assemble sub-structures to limit the onset of surface defects.

**3 - 3:20 pm**

**3435833: Environmental Effects on Friction of Graphene Step Edges**

Zhe Chen, Seong Kim, Pennsylvania State University, University Park, PA

Graphene is an ideal material for lubrication coatings. However, graphene step edges, which are nearly inevitable on the graphene coating, have a much higher friction than the graphene basal plane and thus

deteriorate the overall lubricity of the coating. In this work, the friction properties of a single layer graphene edge on highly oriented pyrolytic graphite (HOPG) are investigated with atomic force microscopy (AFM). It is found that distinct friction behaviors can be obtained in various environmental conditions. The adsorption isotherm of vapor molecules on HOPG surface is studied. Then, the friction mechanism is discussed. This work enriches the understanding of frictional properties at atomic step edges and is helpful for the application of 2D materials as lubrication coatings.

**3:20 – 4 pm - Meet The Experts**

Tuesday, November 10, 2020

**9 – 9:55 am - Keynote Presentation**

Rosa Espinosa-Marzal, University of Illinois at Urbana-Champaign

***Modulating Slip, Adhesion and Friction of Graphene Via Substrate-Induced Doping***

3A

Virtual Breakout Room 1

**Tribochemistry I**

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**Session Chair:** Wilfred T. Tysoe, UW Milwaukee, Milwaukee, WI

**10 - 10:20 am**

**3423181: Influence of Rubbing Material on ZDDP Tribofilm Formation**

Mao Ueda, Amir Kadiric, Hugh Spikes, Imperial College London, London, United Kingdom

In recent years the role of zinc dialkyldithiophosphate (ZDDP) as an antiwear additive in engine oils has become increasingly important because of the use of low viscosity oils to improve fuel economy. Such low viscosities mean that engine components operate for longer periods in thin film mixed lubrication conditions where wear may occur. Although a great deal of research has been carried out on ZDDP tribofilm on steel substrate, the understanding of tribofilm formation on non-ferrous substrates is limited. It has recently been shown that ZDDP tribofilms on steel can have either a nanocrystalline or amorphous structure and that tribofilms with a nanocrystalline structure are more durable than amorphous ones. This presentation describes the influence of rubbing material, including non-ferrous surfaces, on ZDDP tribofilm formation and investigates the relationship between tribofilm properties and durability on these surfaces.

**10:20 - 10:40 am**

**3439423: Adsorption on Metal Oxides: An in Silico Design of Lubricants**

Sarah Blanck, Sophie Loehle, Centre de Recherche Total de Solaize, Solaize, France, Carles Marti, Carine Michel, Stephan Steinmann, Laboratoire de Chimie ENS de Lyon, Lyon, France

Lubrication plays a major role in a wide range of key sectors from motors to metal working. Changes in formulations can lead to modifications of the wettability and the tribological properties. Therefore, it is important to better understand the interactions between the lubricant and the surface. Computational chemistry based on density functional theory was shown to be a powerful tool to describe those interactions. Here, we have determined the influence of different types of additives in the wetting process, by comparing their adsorption energies with their solvation energies in a model lubricant base oil [1]. As the additives are often large multifunctional molecules, we developed an automated workflow DockOnSurf to determine the most favorable adsorption site on both the molecule and the surface, as well as the most favorable conformation for the molecule. The possibility of film formation was also considered. [1] S. Blanck et al., Tribology International 2020, 145, 106140.

**10:40 - 11 am**

**3432543: Understanding the Effect of Forces on Tribochemical Reactions**

Wilfred Tysoe, Alejandro Boscoboinik, UW Milwaukee, Milwaukee, WI

The effect of applied stress on the rates of mechano- or tribochemical reactions is conventionally described using the Bell model where the stress-induced reaction rate varies as  $\exp(\sigma\Delta V^\ddagger/k_B T)$ , where  $\sigma$  is the applied stress,  $k_B$  is the Boltzmann constant,  $T$  the absolute temperature and  $\Delta V^\ddagger$  is the activation volume. Strategies for measuring reaction pathways and their kinetics are illustrated using the gas-phase lubrication of copper by dimethyl disulfide. The tribochemical decomposition of adsorbed methyl thiolate

species is investigated in ultrahigh vacuum. The rate of tribochemical decomposition of methyl thiolate species on a Cu(100) single crystal substrate is accurately measured in ultrahigh vacuum by exerting the force using an atomic force microscopy tip. The results are analyzed using first-principles quantum calculations and the results agree well with experiment. The physical insights obtained using quantum calculation enable precise analytical models to be developed for tribochemical reaction rates.

## **11 - 11:30 am - Meet The Experts**

**11:30 - 11:50 am**

### **3432627: Formation of Metastable Phases in Tribochemical Reactions**

Wilfred Tysoe, Resham Rana, UW Milwaukee, Milwaukee, WI

The tribochemical decomposition of methyl thiolate species on a copper substrate measured on a clean copper sample proceeds via two stress-activated processes. The first is the tribochemical decomposition of adsorbed methyl thiolate species to form gas-phase hydrocarbons and chemisorbed sulfur, followed by an unusual process in which the resulting surface sulfur is transported into the subsurface region of the copper to form a metastable copper sulfide phase. It is found that the transport kinetics depend on the temperature at which the copper was annealed prior to the experiment, and is thus also dependent on the copper crystal size. A depth profile of a focused ion beam (FIB) prepared sample reveals presence of some sulfur in the crystalline regions of the sample, but with preferential sulfur diffusion to the grain boundaries, implies that sulfur surface-to-bulk transport is facilitated by the diffusion of sulfur along grain boundaries that are formed during sliding.

**11:50 am - 12:10 pm**

### **3436574: Stress-Dependent Adhesion in Nanoscale Contacts**

Tevis Jacobs, Sai Vishnubhotla, Andrew Baker, University of Pittsburgh, Pittsburgh, PA, Rimei Chen, Ashlie Martini, University of California, Merced, Merced, CA

Contact mechanics models are extensively used to describe, measure, and predict the properties of nanoscale contacts. An important assumption in these models is that the work of adhesion is constant for a given pair of materials. Recent studies (Milne et al., ACS AMI, 2019 and Vishnubhotla et al., Tribol. Lett., 2019) have shown that this assumption can break down for silicon-diamond contacts, and the work of adhesion can vary with stress. Here, we have conducted more than 70 in situ transmission electron microscopy and molecular dynamics simulation tests to investigate the effect of compressive pressures up to 25 GPa. We have also investigated other covalently-bonded systems to understand the universality of these trends. The results demonstrate how the loading modifies the atomic-scale surface interactions that determine adhesion.

**3B**

Virtual Breakout Room 2

## **Surface & Interfaces III**

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**Session Chair:** Seong Kim, Pennsylvania State University, State College, PA

**Session Vice Chair:** Talia Sebastian, Department of Defense, Warren, MI

**10 - 10:20 am - CANCELLED**

### **3439269: The Necessary Condition for a Hard Coating to Strengthen a Coated Sphere**

Zhou Chen, State Key Laboratory of Fluid Power and Mechatronic Systems, Zhejiang University, Hangzhou, China and

A finite element analysis is performed to study the yield resistance of a coated sphere subjected to normal contact loading. Moderately hard coatings that were omitted in previous literature are considered. A maximum weakening/strengthening effect of minimizing/maximizing the yield resistance is observed to

be linked to the transition of yield inception location. Three types of such links are revealed, two of which are associated with moderately hard coatings. The necessary condition for a hard coating to strengthen a coated sphere is proposed. Only hard coatings with yield strength ratio above a threshold value is able to provide a constructive strengthening effect. For some commonly used substrate materials in practical engineering, the admissible hard coatings include some of the moderately hard coatings.

**10:20 - 10:40 am**

**3439437: Insights into the Formation of Protective Tribo-Layer on Ti6Al4V in the Simulated Body Fluid Environment**

Jiahui Qi, Mark Rainforth, University of Sheffield, Sheffield, United Kingdom

Ti-6Al-4V has been used as the surgical implant material for long time because of its good strength-to-weight ratios, corrosion resistance and bioavailability. The tribo-corrosion property and the formation of the tribo-layer in simulated body fluid condition with different surface charges has been studied in current study. To unpuzzle the complicated nature of the dynamic formation process, high resolution TEM, STEM EELS have been used to characterise the structure and chemical composition the tribo-layer. Micro-mechanical property was tested by Micro-pillar compression. Geometrically necessary dislocations (GND) density was calculated via TEM and precession electron diffraction (PET), which shown an enhanced microstructure of the subsurface under wear track.

**10:40 - 11 am**

**3435997: Development of a ReaxFF Reactive Force Field for the Study of Iron Phosphates with Molecular Dynamics**

Talia Sebastian, Department of Defense, Warren, MI, Diana van Duin, Adri van Duin, RxFF Consulting, LLC, State College, PA

Metal phosphates have been historically used as surface pretreatments for ferrous materials to prevent corrosion and improve adhesion of subsequent coatings. Recently however, a renewed interest into their material and surface chemistry properties for other applications has been witnessed. To improve our fundamental understanding of their complex material and surface chemistry, we have developed a ReaxFF reactive force field for the molecular dynamics study of iron phosphates specifically, by optimizing existing phosphate and iron oxide ReaxFF parameters to newly derived DFT parameters for bulk and molecular iron phosphate systems, as well as those for iron phosphate surface and hydrolysis chemistry. The ReaxFF reactive force field was validated through simulations of iron phosphates in gaseous, aqueous, and organic environments. Thus, we present a ReaxFF reactive force field that is a highly versatile molecular dynamics tool and transferable to the study of a wide range of materials.

**11 - 11:30 am - Meet The Experts**

**11:30 am - 12:10 pm**

**3439430: "SPOTLIGHT" - Chemical and Physical Origins of Friction on Two-Dimensionally Flat Surface with Atomic Steps**

Seong Kim, Pennsylvania State University, State College, PA

When two solid surfaces are in contact and shear each other, there is always a friction. Depending on the materials involved and the chemistry of surrounding environments, friction coefficient can be even larger than 1 or as small as  $<0.01$ . What governs such a large variance in friction coefficient? To better understand the origins of friction, we studied friction on a chemically and topographically well-defined interface  $\blacklozenge$  a graphite step edge  $\blacklozenge$  using atomic force microscopy and molecular dynamics simulations. We identified the separate contributions of physical and chemical processes to friction and showed that friction coefficient can be separated into two terms corresponding to these effects. We also found that the friction force measured with an AFM tip moving across an atomic step edge does not positively correlate with the adhesion force measured with the same tip at the same step edge. The findings provide deeper insights into the chemical and topographic origins of friction.

## Lubricants I

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**Session Chair:** Demófilo Maldonado Cortés, Universidad de Monterrey, Monterrey, Mexico

**10 - 10:40 am**

**3435312: "SPOTLIGHT" - Mechanochemistry at Diamond-Rock Interfaces**

Jagjeevan Bhamra, James Ewen, Daniele Dini, Imperial College London, London, United Kingdom, Marc Bird, John Bomidi, Baker Hughes, Houston, TX

The interactions between polycrystalline diamond compact (PDC) drill bits and rock-surfaces is not fully understood. We perform molecular simulations to investigate the interactions in diamond-rock systems. We use nonequilibrium molecular dynamics (NEMD) simulations to explain the increased friction properties observed experimentally at diamond-calcite interfaces compared to diamond-quartz. We consider both dry and aqueous environments using new reactive force field (ReaxFF) parameters, which have been verified against first principles calculations. We monitor mechanochemical processes within these systems such as tip-substrate bond formation and structural changes within both the tip and the substrates. These successfully rationalise the experimentally-observed tribological behaviour.

**10:40 - 11 am**

**3439432: Base Oil, Ionic Liquid, Anti-Wear Additive, and Friction Modifier ♦ Which One is at the Solid/lubricant Interface?**

Seong Kim, Pennsylvania State University, State College, PA

Lubricants are not a single component liquid; they are a mixture of various additives in base oil. Then, a fundamental surface science is which component is present at the solid/lubricant interface? We studied this question using sum frequency generation (SFG) spectroscopy for lubricants containing ionic liquids ([P8888][DEHP] and [N888H][DEHP]), ZDDP (anti-wear additive), and organic friction modifiers (OFM) in PAO base oil. The SFG analysis results showed that the air/liquid interface is always dominantly populated by PAO due to its lower surface tension in comparison to ionic liquids, modifiers and additives. However, at the silica/liquid interface, it was found that [P8888][DEHP] strongly adsorbs to the silica surface from all mixtures with PAO and organic friction modifier (OFM); adsorption of [N888H][DEHP], however, is insignificant at the same conditions. Results from this study reveal the compatibility among ionic liquids, ZDDP, organic friction modifier and base oil.

**11 - 11:30 am - Meet The Experts**

**11:30 - 11:50 am**

**3413733: Oxidative Stability of Estolides**

Mark Miller, Debby Neubauer, Biosynthetic Technologies, Indianapolis, IN

A set of base oil samples, including estolides, esters, PAGs, PAOs, and mineral oils were tested for their resistance to oxidation, according to the industry standard RPVOT test (ASTM D2272). The raw data from these experiments suggest that the RPVOT method underestimates the oxidative stability of estolides and esters relative to the other base oils tested. Different oxidative stability methods were also explored and a comparative analysis was performed.



**11:50 am - 12:10 pm**

**3439426: Designing a Simple Test to Measure Lubricant Efficiency**

Marc Ingram, Ingram Tribology Ltd, Carmarthen, United Kingdom, Izzy Roots, Clive Hamer, PCS Instruments, London, United Kingdom

The ability of a lubricant to reduce friction and increase efficiency is one of its key functions. However, a standardized lab scale efficiency test for lubricants does not exist. In this work we take a common tribometer and design a test sequence to allow the efficiency rating of any lubricant to be quickly and accurately measured. The user simply enters the KV40 and KV100 value for the lubricant being tested. The test software then calculates the entrainment speeds to maintain the same test severity for each lubricant, regardless of viscosity. Lubricants are then rated for efficiency in terms of their ability to maintain low friction in the boundary, mixed and EHD regimes, using data from the normalized Stribeck curves. The method is being designed with repeatability in mind, across the entire range of common lubricant grades. This new method simplifies efficiency measurement, helping the development and qualification of new lubricants.

**12:10 - 12:30 pm**

**3439428: Development of a Fired-Engine Test Cycle to Evaluate the Effect of Engine Oil Formulation on Emulsion Formation**

Dan Engstrom, Southwest Research Institute, San Antonio, TX

With the growth of hybrid vehicles in the market, there is increased concern regarding the formation of water-in-oil and fuel-in-oil emulsions due to the absence of sustained engine operation. In hybrid or plug-in hybrids, the electric drive system provides much of the power needed for low speed commuting cycles and fails to allow the oil to heat up as it would in a conventional IC engine-powered vehicle. The suggested solution when emulsions form is to drive the hybrid vehicle on the highway to heat the oil to standard operating temperature to evaporate the water and fuel in the oil. Due to a desire to better understand this phenomena and evaluate the performance of different oil formulations, a two-stage test development was selected. The study described outlines the first stage of development with a modified Sequence VH stand demonstrating the repeatable formation of emulsions with a baseline oil and studying the effects of engine oil formulations on reducing such emulsion.

**12:30 – 1 pm - STLE Connect (Exhibits & Posters)**

**1 – 1:55 pm - Keynote Presentation:**

Jean-Francois Molinari, EPFL, Switzerland

***Revisiting Archard's Wear Model: A Dialog Between Scales***

**4A**

**Virtual Breakout Room 1**

**Tribochemistry II**

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**Session Chair:** Seong Kim, Pennsylvania State University, University Park, PA

**2 - 2:40 pm**

**3438144: "SPOTLIGHT" - Understanding the In-Situ Formation and Evolution of Phosphorus Antiwear Tribofilms with FFM and NanoIR-AFM**

Kerry Cogen, Infineum USA L.P., Linden, NJ, Alison Pawlicki, Matthias Lorenz, Nickolay Borodinov, Olga Ovchinnikova, Oak Ridge National Laboratory, Oak Ridge, TN

In vehicle transmissions, antiwear tribofilms form from lubricating fluids on rolling / sliding contacting surfaces and serve to control friction and protect surfaces from wear and fatigue. Understanding the mechanism of antiwear film formation and how to tune surface chemistry to control functionality is

essential for development of next generation transmission fluids. Here, we developed a unique multimodal AFM methodology to understand initial film formation from different phosphorus-containing lubricants in-situ. We combined Friction Force Microscopy (FFM) to capture the spatial details of friction over the surface as the tribofilm forms and evolves and Nano Infrared Spectroscopy AFM (NanoIR-AFM) to understand the chemistry of the film. We demonstrate the formation of antiwear tribofilms on steel surfaces, the effect of lubricant formulation on how these films evolve in-situ, and the differences in chemistry between these films.

**2:40 - 3 pm**

**3439439: Tribological and Tribochemical Evaluation of Various Lubricants on Steel as well as WC-DLC Coating under Extreme-Pressure Boundary Lubrication Conditions: Rig Test: Part 2**

K.K. Mistry, The Timken Company, North Canton, Ohio

Diamond-like carbon (DLC) coating has demonstrated excellent results for sliding-rolling contact parts, especially for the components subjected to extreme pressure conditions and severe boundary lubrication. The coating help to increase scuffing load capacity and prolong component durability. The commercially available lubricants (oils and greases) are compatible with ferrous surfaces, but normally have not been optimized for coatings. In the present work, the tribological properties of tungsten carbide doped DLC (WC-DLC) against steel ball with various lubricants in boundary lubrication conditions have been evaluated on bench & rig test. The effect of lubricant was correlated with the wear performance. The wear measurements were conducted at small time-intervals along with the examination of the chemistry of the tribofilm using surface sensitive techniques: XPS and SEM/EDS. The surface reactions between the additive-coating surface significantly influence its tribological performance.

**3 - 3:20pm – Open Slot**

**3:20 - 4 pm - Meet The Experts**

**4B**

Virtual Breakout Room 2

**Surfaces & Interfaces IV**

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**Session Chair:** Mehmet Baykara, University of California Merced, Merced, CA

**Session Vice Chair:** Mahyar Sfsnar Mohajer, University of Arkansas, Fayetteville, AR

**2 - 2:20 pm**

**3468267: Metrology and Numerical Characterization of Random Rough Surfaces - Data Reduction via an Effective Filtering Solution**

Itzhak Green, GA Tech, Atlanta, GA

To study surface topography, synthetic surfaces are generated herein using a harmonic waveform precisely as McCool had done. However, here the signals are contaminated by a white noise process with various magnitudes. A signal to noise ratio is defined and used to assess the quality of the signal, and the spectral moments are evaluated for various magnitudes of the noise. Since closed-form solutions are available for the spectral moments of the uncontaminated signal, the contaminated signals are evaluated vis-à-vis the exact anticipated values, and the errors are calculated. It is shown that using the common techniques (such as those outlined by McCool) can lead to enormous and unacceptable errors. Resolution is studied as well; it is shown to have an effect only in the presence of noise, but by itself it has no independent influence on the spectral moments. A generalized exponential smoothing filter, G-EXP, is constructed, and it is shown to markedly moderate the errors and reduce them to acceptable levels, while effectively restoring the underlying surface physical characteristics. Moreover, the filtered signals do not suffer from resolution problems, where results, in fact, improve with higher (i.e., finer) resolutions. Fractal-

generated signals are likewise discussed.

**2:20 - 2:40 pm**

**3436700: Nanoparticle  $\alpha$ -ZrP Enhanced Super Hydrophobicity**

Yan Chen, Xuezheng Wang, Abraham Clearfield, Hong Liang, Texas A&M University, College Station, TX

A surface coating made of nanoparticle  $\alpha$ -ZrP was synthesized using one-step drop cast processing. The coating consisted of surface modified  $\alpha$ -ZrP nanoparticles of 3 different sizes. Characterization was conducted using an atomic force microscope (AFM) and a goniometer. Results showed that the aggregation of nanoparticles resulted in a dual distribution of surface roughness leading to superhydrophobicity with contact angle up to  $160^\circ$  against de-ionized water. Two factors enable super hydrophobicity, hydrophobic  $\alpha$ -zirconium phosphate nanoparticles and self-assembly into dual model distribution. The dual model distribution of the surface was formed by the fractal clustering of nanoparticles and the platelet shaped nanoparticles' random orientation.

**2:40 - 3 pm**

**3440136: Tribology of Surfaces with 3D Textures Fabricated via Two Photon Lithography: A Multi-Scale In-Situ Study**

Mahyar Afshar Mohajer, Min Zou, University of Arkansas, Fayetteville, AR

Reducing real area of contact via surface texturing is an effective way to decrease adhesion and friction between two surfaces in dry rubbing conditions. Enabled by a high-resolution additive manufacturing technique known as Two Photon Lithography (TPL), surface textures were fabricated with precise shape, position, and sub-micron dimension control. This allows a systematic study of textures with truly 3D structures (cones) versus equivalent 2.5D structures (rods and cylinders). An in-situ multi-scale tribological study of the textures was carried out using a digital microscope with a tribometer at the macro-scale and an in-situ SEM picoindenter at the micro-scale. Cone textures not only had the lowest friction due to the lowest area of contact at the tip but also had the best durability provided by a large base. In-situ observations provided valuable insights at different scales such as the relationship between structure deformation and friction at micro-scale.

**3 - 3:20 pm**

**3454134: Direct Imaging of Atomic-Scale Ripples on  $\text{MoS}_2$  and Their Effect on Friction Anisotropy**

Mehmet Baykara, Ogulcan Acikgoz, University of California Merced, Merced, CA, Omur Dagdeviren, Peter Grütter, McGill University, Montreal, Quebec, Canada

Theory predicts that two-dimensional (2D) materials may only exist in the presence of out-of-plane deformations on atomic length scales, frequently referred to as ripples. While such ripples can be detected via electron microscopy, their direct observation via surface-based techniques and characterization in terms of interaction forces and energies remain limited, preventing an unambiguous study of their effect on tribological characteristics, including but not limited to friction anisotropy. Here, we employ high-resolution atomic force microscopy to demonstrate the presence of atomic-scale ripples on supported samples of few-layer molybdenum disulfide ( $\text{MoS}_2$ ). Three-dimensional force / energy spectroscopy is utilized to study the effect of ripples on the interaction landscape. Friction force microscopy reveals multiple symmetries for friction anisotropy, explained by studying rippled sample areas as a function of scan size. Our experiments contribute to the continuing development of a rigorous understanding of the nanotribology of 2D materials.

**3:20 - 4 pm - Meet The Experts**

## Lubricants II

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**Session Chair:** Laura Peña Parás, Universidad de Monterrey, Monterrey, Mexico

**2 - 2:20 pm**

**3428676: Observation of Polymer Orientation in Oil under High Shear**

Tatsuya Kusumoto, Moritsugu Kasai, Idemitsu Kosan Co.,Ltd, Ichihara-Shi, Japan, Mikihiro Takenaka, Kyoto University, Kyoto, Japan

We firstly have succeeded in visualizing the molecular orientation of viscosity index improver (polymer) in engine oil under high shear rate in-situ. Fluid resistance and oil film formation on lubrication surface in engine oil are important issues to improve the performance of engine oil. The measurement of the viscosity of the engine oil with polymer is not enough to clarify the fluid resistance and oil film formation and realized the molecular orientation of the polymers in the oil is an important factor for the phenomena. We thus developed the novel cell (Fig.1) which enables to measure small-angle X-ray scattering (SAXS) under high shear rate and measured the molecular orientation in the cell by using synchrotron SAXS method at SPring-8, Japan. The radius of gyration in the flow direction was 17.3 nm, and the radius of gyration the direction perpendicular to the flow was 16.0 nm (Fig.2), indicating that the polymers elongated to the flow direction under high shear rate.

**2:20 - 2:40 pm - CANCELLED**

**3390912: Effects of Lubricant Additives on Hydrogen Permeation under Rolling Fatigue**

Yoji Sunagawa, Idemitsu Kosan Co.,Ltd, Ichihara, Chiba, Japan

In rolling bearings used in automotive power transmission parts such as Continuously Variable Transmission and wind turbines, early bearing failure accompanied by white microstructures below the raceway subsurface occurs. The main cause is often thought to be the effect of hydrogen embrittlement. Hydrogen embrittlement is the process by which steel materials become brittle and fracture due to the introduction and subsequent diffusion of hydrogen into the metal. In rolling bearings, since active nascent metal surface is exposed, lubricant oils between metal surfaces is decomposed, and hydrogen is generated and penetrates into steels. This study describes the effects of lubricant additives on the permeation of hydrogen into AISI 52100 bearing steel in rolling contact. Lubricated tests were conducted in a nitrogen atmosphere. PAO was used as the base oil. Sample A and sample B were formulated with representative detergent additives. Oil decomposition test and rolling contact fatigue test were conducted.

**2:40 - 3 pm**

**3415767: Tribological Performances of 3-(Trimethylsilyl)-1-Propanephosphate Anion Based Ionic Liquids as Lubricant Additives**

Shouhei Kawada, Shinya Sasaki, Masaaki Miyatake, Tokyo University of Science, Tokyo, Japan, Gen Masuda, Nisshinbo Holdings, Inc., Chiba, Japan

Ionic liquids are expected to be used as novel lubricant additives. They are salts that exist as liquid phase at room temperature. This investigation synthesized ionic liquids with new anionic structure, and evaluated their tribological performances as lubricant additives. This investigation used three types of ionic liquids (tributyl-dodecylphosphonium 3-(trimethylsilyl)-1-propanephosphate ([BDDP][SiC3P]), tributyl-hexadecylphosphonium 3-(trimethylsilyl)-1-propanephosphate ([BHDP][SiC3P]) and trihexyl-tetradecylphosphonium 3-(trimethylsilyl)-1-propanephosphate ([HTDP][SiC3P])) as lubricant additives. All ionic liquids exhibited low friction coefficients as compared with neat base oil. This silicon-containing phosphate anion can be expected as lubricant additives that provide a high friction reducing effect.

**3 - 3:20 pm - CANCELLED**

**3419906: Tribological Performance of Piston Compression Ring in Artificial Intelligence Based Design Green Lubricant during Cold Start-Up**

Imran Shahid, HITEC University, Taxila, Punjab, Pakistan

This work presents the amount of loss of energy to overcome friction of piston rings and design of hybrid nano-fluids based on Artificial Neural Network during cold-start-up. The input feature parameters are load, concentration, speed, and concentration, and output parameter is Coefficient of Friction (COF). Customized ANN was developed and pin on disc experimental data generated is used for training the model. New hybrid nanofluid was developed having better tribological properties by computational technique. Multi-physics numerical simulations were conducted on compression ring during cold start-up by combining the piston ring dynamic model with lubrication model for hybrid nano fluid and mineral oils. The development of film thickness, frictional force and power loss are studied during each cycle. Comparative analysis of the numerical simulation results was conducted to evaluate the performance of hybrid nanofluids and mineral oils. Results showed that Artificial Intelligence based lubricant has 45-51% less COF than mineral oil.

**3:20 – 4 pm - Meet The Experts**

8 am – 12 pm - ASME Course  
(Separate Registration Required)

5A

Virtual Breakout Room 1

## Materials Tribology I

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**Session Chair:** Tevis Jacobs, University of Pittsburgh, Pittsburgh, PA

**9 - 9:20 am**

**3414131: Deformation Mechanisms and Friction of High-Purity Copper during Sliding**

Christian Haug, Friederike Ruebeling, Ankush Kashiwar, Peter Gumbsch, Christian Kübel, Christian Greiner, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Understanding the mechanisms governing dislocation-mediated plastic deformation and friction at metal sliding interfaces may greatly help expedite the development of materials tailored for low friction and little wear. This work investigates the microstructural changes induced by sliding on high-purity copper in the vicinity of a twin boundary. The formation of two distinct horizontal line features (dislocation trace lines, DTL) is observed. Their interaction with the twin boundary is studied using automated crystal orientation mapping (ACOM). Three concurrent fundamental deformation mechanisms are discerned: A simple shear process of the subsurface area, a localized shear process at the lower DTL and a crystal rotation at the DTLs. Further analysis by electron diffraction elucidates the influence of parameters such as crystallographic orientation and load regime on these processes. The interdependence of deformation and friction is demonstrated by corresponding friction measurements.

**9:20 - 9:40 am**

**3431532: Effect of Temperature and Filler on the Tribological Responses of Sintered Polyimides**

Kian Kun Yap, Marc Masen, Imperial College London, London, South Kensington, United Kingdom

A metal-polymer sliding interface can self-lubricate due to the transfer film formation mechanism. This makes it ideal for high-temperature applications where liquid lubricants are not applicable. Although the transfer film formation of PTFE has been investigated in detail by researchers, that of most other polymers remain unclear. Hence, high-temperature polyimide (PI)/AISI 52100 sliding tests were carried out to study how different surface temperatures and filler's contents control the tribological responses. In general, the role of temperature is more dominant than that of filler in governing the tribology of PI. Temperature changes the thermochemistry of PI and then alters the characteristics of transfer materials, namely thickness, orientation, percent coverage, and stability. Then, these affect the friction coefficient,  $\mu$ , sliding fluctuation,  $\sigma$ , and wear rate,  $w_s$  of the system. In brief, the sliding of PI with 40 wt% graphite at 280 degrees Celsius gives the lowest  $\mu$ ,  $\sigma$ , and  $w_s$ .

**9:40 - 10 am**

**3435338: Nanoindentation Analysis of Evolved Bearing Steel under Rolling Contact Fatigue (RCF)**

Muhammad Abdullah, Zulfiqar Khan, Bournemouth University, Bournemouth, United Kingdom, Wolfram Kruhoeffer, Schaeffler Technologies AG & Co. KG, Herzogenaurach, Germany

The bearing material operated under RCF is subjected to the triaxial stress state where work hardening followed by softening has been reported under the contact track. Such nonconformities (hardening/softening along with microstructural alterations) create complexities to model the cyclic hardening of bearing material under RCF. Current study presents a semi-empirical approach to evaluate the evolved subsurface response of bearing material with the help of a three-faced pyramidal Berkovich

nanointender employing expanding cavity model for strain hardening materials. The expanding cavity model converts the localized measured hardness change to flow stresses which have been evolved during strain-hardening and microstructural phase changes of the bearing material. Moreover, to evaluate the representative stress-strain curve of the altered microstructure, a 5um spherical indenter was employed in a cyclic loading manner. The use of the spherical indenter with the integration of Field and Swain numerical model enables to extract the representative flow curve of the material at highly localized areas which cannot be possible even with miniature uniaxial tension/compression test.

**10 - 10:20 am**

**3416413: Maximizing the Impact of Nanofillers on PTFE Wear Resistance**

Istiaque Alam, David Burris, University of Delaware, Newark, DE

Certain alumina filler reliably reduces wear of polytetrafluoroethylene (PTFE) by 99.9%. What makes these microscale aggregates of nanofillers unique is their ability to survive processing and subsequently disrupt sub-surface damage in the nanocomposite while promoting favorable tribochemical reactions after disbanding at the sliding interface. This strength, however, reveals a limitation: any particle performing two functions excels at neither. This paper uses a hybrid (PEEK microfiller + alumina nanofiller) approach to separate these functions and isolate the minimum effective dose of nanofillers. Outsourcing the function of mechanical reinforcement to the PEEK revealed that the optimal nanofiller content is at least 10X below the 2-15 wt% optima reported in virtually all other polymer nanocomposite wear studies; hybrid design appears necessary to extract the full benefit of nanofillers in this context.

**10:20 - 10:40 am - Break**

**10:40 - 11 am**

**3407025: Wear Effects from Binary and Ternary Mixtures of Methyl-Esters in Mineral Oil**

Gustavo Molina, John Morrison, Emeka Oniejizu, Valentin Soloiu, Georgia Southern University, Statesboro, GA

Previous research showed that oil dilution by biodiesels, which occurs in engines because of unburned biofuel leaking to the oil-pan, can enhance degradation of engine-oil lubricity. Research is presented on tribological effects on SAE 1018 steel when tested with mixtures of pure methyl-esters in SAE 15W40 mineral oil. Two diluting biodiesels (Soybean-oil- and Peanut-oil-biodiesel), and six typical methyl-ester biodiesel components (Methyl-Palmitate, -Oleate, -Stearate, -Linoleate, -Laurate and -Myristate) at six different dilution ratios, were tested in two different tribometers. The results suggest that the testing of just pure methyl-esters as oil-diluting fractions would not fully explain the lubricity changes observed for biodiesel-in-oil mixtures, and ongoing preliminary testing with ternary mixtures (i.e., of two typical methyl-esters in oil) is discussed.

**11 - 11:20 am**

**3422696: On Measuring the Friction Component of Oils**

Kenneth Budinski, Bud Labs, Rochester, NY

There is worldwide interest in reducing energy consumption and this project addresses the question: do different oils produce different friction results in the same tribosystem. Is one oil more "slippery" than another? Initial testing with an inclined plane test (ASTM G 214) suggested that higher viscosity fluids produce lower breakaway friction. Bushing vs. shaft tests at three velocities suggested that bearing torques were the same for oils ranging from 0 weight to 40 weight. The overall conclusions of these tests are that oils may have different breakaway friction characteristics under boundary lubrication conditions, but system friction becomes the same under full-film lubrication conditions. In these studies, system friction did not decrease with speed as predicted by the Stribeck curve.

**11:20 - 11:40 am**

**3436076: A New Test Method for Direct Measurement of Friction in Biomass Material**

Maria Cinta Lorenzo Martin, Oyelayo Ajayi, George Fenske, Argonne National Laboratory, Argonne, IL,

Jordan Klinger, Yidong Xia, INL, Idaho Falls, ID, Troy A. Semelsberger, NREL, Golden, CO

The reliable and controlled flow of solid particulate biomass materials from bins, hoppers, etc. is essential for successful operation in every biorefinery. Friction is one of the critical material properties governing the flow of biomass materials and an important input into material handling equipment design. The current approach by industry to assess friction is different variants of shear testing. A new test method was developed and demonstrated to directly measure the particle-particle friction in biomass materials. A bench top tribometer was adapted to measure friction of biomass materials by attaching copious amount of biomass materials unto sliding surfaces. The pressure within the biomass during friction measurement was mapped using a pressure sensitive film technique. The new friction measurement method was demonstrated for two different biomass materials, namely grass and pine wood chips.

**11:40 am - 12:00 pm**

**3436081: Tribological Performance of PDA+PTFE Coating in Oil-Lubricated Condition**

Sujan Ghosh, Min Zou, University of Arkansas, Fayetteville, AR

In this study, the coefficient of friction and wear properties of spray-coated,  $45\pm 3$   $\mu\text{m}$  thick PTFE and PDA+PTFE coating on cast iron substrate were investigated in oil-lubricated conditions. Tribological test results showed that the PDA+PTFE coating lasted 13,667 s, which is five times higher than the PTFE coating. The PTFE and PDA+PTFE coating both showed lower COF in oil-lubricated condition compared to the COF of PTFE in dry condition. The addition of PDA in PTFE increased the modulus of elasticity and adhesion of the PTFE coating from 0.61 GPa to 0.97 GPa, and 154 nN to 172 nN, respectively. The higher modulus of elasticity was responsible for the enhanced durability of the PDA+PTFE coating compared to that of the PTFE coating. The better nanomechanical properties, cross-linking of the PTFE and PDA particles, and better load carrying capacity were responsible for the better durability of the PDA+PTFE coating in oil-lubricated conditions.

5B

Virtual Breakout Room 2

**Surfaces & Interfaces V**

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**Session Chair:** Gus Greenwood, University of Illinois at Urbana-Champaign, Urbana, IL

**Session Vice Chair:** Filippo Mangolini, The University of Texas at Austin, Austin, TX

**9 - 9:20 am**

**3439434: Exploring Tunable in situ Doping of Single Layer Graphene through Nanotribology**

G. Greenwood, J. Kim, S.M. Nahid, S. Nam, R.M. Espinosa-Marzal, University of Illinois at Urbana-Champaign, Urbana, Illinois

Graphene's theorized and reported low friction makes it a promising candidate for a solid lubricant, yet graphene has relevant tribological characteristics beyond low friction. Of particular note is a phenomenon commonly referred to as doping, where graphene's surface properties are affected by both the substrate it is supported by and the environment it is in contact with. Our previous work has demonstrated differences in graphene's nanotribology driven by changes in the substrate, indicating that selectively choosing graphene's supporting substrate is an avenue for tuning a system's tribology. Changing the substrate, however, is a labor-intensive process for repeated experiments and also has the potential to complicate nanoscale measurements. In this work we present an in-development method to control the doping of graphene by leveraging a sample construction similar to a field effect device, eliminating the need for many different graphene samples with different doping states. The setup is easily usable in most instruments, allowing in situ changes to the doping state. We expect this method to drive further investigation into the nanotribological properties of graphene.



**9:20 - 10 am**

**3439419: "SPOTLIGHT" - In Situ Study of the Lubrication Mechanism of Phosphonium Phosphate Ionic Liquid in Nanoscale Single-Asperity Sliding Contacts**

Filippo Mangolini, Zixuan Li, Oscar Morales-Collazo, Hugo Celio, Andrei Dolocan, Robert Chrostowski, Joan Brennecke, The University of Texas at Austin, Austin, TX, Jerzy Sadowski, Brookhaven National Laboratory, Upton, NY

Phosphonium phosphate ionic liquids (PP-ILs) have attracted considerable attention in tribology owing to their high thermal stability, good miscibility in hydrocarbon fluids, and excellent lubrication performance. Despite the scientific weight of previous macroscale tribological studies of PP-ILs, a fundamental understanding of the nanoscale lubrication mechanism is still lacking. Here, we used atomic force microscopy (AFM) to evaluate the processes occurring at sliding interfaces in situ, in single-asperity contacts. The AFM experiments, in which a diamond tip was slid on steel in PP-IL, indicated a reduction in friction only after the removal of the native oxide layer from steel. Based on laterally-resolved ex situ analyses of the surface chemistry of steel by X-ray photoemission electron microscopy, low energy electron microscopy, and time-of-flight secondary ion mass spectrometry, a phenomenological model will be proposed to account for the observed tribological behavior.

**10 - 10:20 am – Break**

**10:20 – 10:40 am**

**3489786: The Origin of Surface Damage and its Link to Microstructure - A Journey Through Recent Modelling and Theoretical Advances**

Daniele Dini, Imperial College of London, London, United Kingdom

Microstructural variation in samples subjected to tribological loads has commonly been observed in experimental studies for various crystalline metals, including nickel, copper and aluminum. Numerical investigations spanning many length- and time-scales, ranging from atomistic to discrete dislocation plasticity (DDP) and crystal plasticity (CP), have been performed to understand surface and subsurface modifications under sliding. However, due to the complexity of the systems under investigation, neither experimental nor numerical studies have yet been able to elucidate all the mechanisms responsible for plastic deformation and material damage leading to e.g. wear. This presentation summarises recent modelling advances made to underpin the mechanisms responsible for microstructural evolution, including the unravelling of lattice rotation responsible for dislocation tracelines using the DDP framework and the mapping of deformation mechanisms of binary alloys using atomistic simulations.

**5C**

**Virtual Breakout Room 3**

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**Tribochemistry III**

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**Session Chair:** James Ewen, Imperial College London, London, United Kingdom

**9 - 9:20 am**

**3439443: In-Situ Reactive Formation of MoS<sub>2</sub> Tribofilms: Interaction with ZDDP and Dispersants**

Manel Rodriguez Ripoll, Bernhard Kohlhauser, Sara Spiller, AC2T research GmbH, Wiener Neustadt, Austria, Carmen Vladu, CEST Centre for Electrochemistry and Surface Technology GmbH, Wiener Neustadt, Austria

In the present work, we study the in-situ reactive formation of MoS<sub>2</sub> tribofilms in lubricated contacts. Instead of using Mo-containing friction modifiers or MoS<sub>2</sub> nanoparticles, we aim to generate MoS<sub>2</sub> in-situ via a tribochemical reaction between sulphur-containing extreme pressure (EP) lubricant additives and molybdenum-containing substrates. MoS<sub>2</sub> formation is verified using Raman spectroscopy and transmission electron microscopy (TEM). Under certain testing conditions, the in-situ tribochemical

formation of MoS<sub>2</sub> is accompanied by the presence of oil-derived carbon tribofilms. In a second step, we address the synergies and antagonisms of the in-situ formed MoS<sub>2</sub> tribofilms with co-additives, such as ZDDP and succinimide dispersants. MoS<sub>2</sub> tribofilms can be tribochemically formed in conjunction with ZDDP tribofilms, as evidenced using TEM. On contrary, the use of dispersants prevents MoS<sub>2</sub> tribofilm formation, analogous to observations done using MoS<sub>2</sub> nanoparticles as lubricant additives.

**9:20 - 9:40 am**

**3438174: Comparing the Composition and Evolution of Macro- and Nano-Scale Phosphorus Antiwear Tribofilms with ToF-SIMS**

Kerry Cogen, Infineum USA L.P., Linden, NJ, Matthias Lorenz, Alison Pawlicki, Nickolay Borodinov, Olga Ovchinnikova, Oak Ridge National Laboratory, Oak Ridge, TN

In vehicle transmissions, antiwear tribofilms form from lubricating fluids on rolling / sliding contacting surfaces and serve to control friction and protect surfaces from wear and fatigue. Understanding the mechanism of antiwear film formation and how to tune surface chemistry to control functionality is essential for development of next generation transmission fluids. Here, we use both macro-scale generation of tribofilms by block-on-ring testing and nano-scale AFM single-asperity experiments for tribofilm preparation, and we analyze the chemical composition of these films by depth profiling Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). We compare macro-scale films prepared from different phosphorus-containing (non-zinc-based) lubricants with variable contact time between the contacting metal surfaces to study changes of the chemical composition of the films formed during their initial formation and evolution. This approach is expected to provide better understanding of the mechanism of early tribofilm formation.

**9:40 - 10 am**

**3439431: Fundamentals of Tribochemistry: Model Study with Tribopolymerization of Adsorbate Molecules**

Seong Kim, Pennsylvania State University, State College, PA

Unlike typical chemical reactions which are initiated by electronic excitation or transition within or among reactant molecules under the influence of heat, light, or electrical bias, tribochemical reactions are initiated by interfacial shear imposed onto the molecules by the solid surface. How could the mechanical energy of solid surfaces be channeled into reaction coordinates of molecules adsorbed and sheared at the sliding interface. We have addressed this question through carefully designed experiments and collaborations with computational groups. This talk will focus on the effects of chemical structures of the adsorbed molecules that are being sheared at the interface as well as the roles of surface chemistry of solid substrates and surrounding gas environments.

**10 - 10:20 am - Break**

**10:20 - 11 am**

**3482237: "SPOTLIGHT" Molecules Under Pressure**

James Ewen, Hugh Spikes, Tom Reddyhoff, Daniele Dini, Imperial College London, London, United Kingdom

High pressures have wide-ranging effects in tribology, from governing the elastohydrodynamic friction of base oils to driving the mechanochemical decomposition of additives. In this talk, we discuss recent high-pressure studies of friction, wear, rheology, and tribochemistry using molecular simulations and specialised experiments. Recent experiments using the Extreme Traction Machine (ETM) have shown that the mechanochemical decomposition and tribofilm formation of zinc dialkyldithiophosphate (ZDDP) under elastohydrodynamic lubrication (EHL) conditions is due to shear stress, rather than hydrostatic pressure. We also discuss how molecular simulations with accurate all-atom force fields can now provide quantitative agreement with high-pressure viscometer measurements for molecular fluids and their binary mixtures. These simulations not only pave the way for accurate in silico prediction of EHL friction, but also provide unique insights into transport behaviour in the high-pressure, supercooled state. Finally, we

discuss molecular fluids that have recently been shown to exhibit macroscale liquid superlubricity under EHL conditions.

6A

Virtual Ballroom

## Cutting Edge Symposium

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**Session Chair:** Nicolas Spencer, ETH, Zurich, Switzerland

**Session Co-Chair:** Wilfred T. Tsoe, UW Milwaukee, Milwaukee, WI

**1 - 1:30 pm**

### **3420392: Prediction of Nanoscale Friction for Two-Dimensional Materials Using a Machine**

#### **Learning Approach**

Prathima Nalam, Behnoosh Sattari Baboukani, Kristofer Reyes, SUNY University at Buffalo, Buffalo, NY, Zhijiang Ye, Miami University, Oxford, OH

Two-dimensional (2D) materials are emerging as alternatives for lubrication additives to control friction and wear in both dry and wet environments. Recent advances in data-driven and computational methods have enabled the discovery of more than 6000 3D materials with potential exfoliation properties, and hence the identification of 2D structures with optimum tribological properties necessitates a machine learning approach.

In this study, we employ Bayesian statistical analysis through the transfer learning approach to predict the maximum energy barrier (MEB) of the corrugated potential energy surface for a wide range of 2D materials. The MEB values predicted for 15 different 2D materials (across two families) while sliding similar layers of a 2D material against each other will enable the development of empirical relations among the descriptors (such as structure, thermal conductivity, etc.) associated with 2D materials and their intrinsic friction property.

**1:30 - 2 pm**

### **3429904: The Influence of Material and Electrical Current on the Formation of Premature Bearing Failures**

Benjamin Gould, Nick Demas, Rober Erck, Maria Cinta Lorenzo Martin, Aaron Greco, Argonne National Laboratory, Chicago, IL

Premature fatigue failures associated with local regions of microstructural degradation (i.e. White Etching Cracks (WECs)) are the predominate mode of failure within wind turbine drivetrain bearings. Although WECs have been reported in the field for over a decade, the conditions leading to this failure, and the process by which this failure culminates, are both highly debated. Recently, it was documented levels of current up to 1A can be measured uptower in turbines. The presented work studies how this variable current effects component failure. The effect of lubricant formulation via variable base fluid and additive composition was also . Moreover, the effect of potential mitigation techniques such as the use of black oxide conversion layers, and other protective coatings will be presented.

**2 - 2:30 pm**

### **3435050: Walking Your Way to Thick Slippery Cartilage**

David Burris, University of Delaware, Newark, DE

The most basic questions about how cartilage and joint function remain unanswered despite nearly a century of research. For example, it is unclear if friction forces are attributable to classical adhesive interactions or fluid shear stresses, if rough interfaces are permeable or impermeable, or if the unusual roughness of cartilage has a purpose. In this talk, I will review our most interesting findings on the topic. I will start by demonstrating that the lubrication is simply proportional to near-surface hydration - as far as we can tell, high friction is impossible on hydrated cartilage surfaces and low friction is impossible on

dehydrated surfaces. Next, I will discuss how cartilage maintains hydration and lubricity despite the leaky nature of the tissue. We show that walking reinflates cartilage and restores lubricity, thickness, and mechanical function. This surprising fact is a bit like driving a car to reinflate a leaky tire. Finally, we will discuss what our measurements suggest about the mechanics of this rehydration process and what it all implies for how we can mitigate our individual risk of cartilage dysfunction and disease.

**2:30 - 3 pm**

**3436427: Graft Copolymers and Bottlebrushes at Surfaces for Tuning Physicochemical and Tribological Properties of Materials**

Edmondo M. Benetti, ETH Zürich, Zürich, Switzerland

The functionalization of inorganic and organic surfaces by highly branched, functional polymer adsorbates enables a fine tuning of the interfacial physicochemical properties and allows one to determine the interaction of the modified support with the surrounding environment. This is valid on metal oxide surfaces, where graft copolymers featuring different compositions and side chain topologies can assemble forming biopassive and lubricious interfaces. Alternatively, from similar inorganic substrates, bottlebrushes with controlled molar mass and side chain length can be grown exploiting controlled radical polymerization (CRP) methods, enabling a broad modulation of steric stabilization of the surface, and tuning its biopassivity and nanotribological properties.

The design concepts and functionalization strategies applied for model inorganic materials can be additionally enlarged to complex tissue surfaces such as articular cartilage, where highly branched, biocompatible copolymers can replace structurally similar biomacromolecules responsible for protection and lubrication of the underlying tissue.

In this contribution, the influence of polymer architecture and composition on the fabrication and properties of graft copolymer- and bottlebrush-based interfaces will be discussed, bringing the above-mentioned cases as examples of highly-technologically-relevant applications.

**3 – 3:30 pm**

**3504881: The Origin of Frictional Energy Dissipation**

J. Frenken, R. Hu, Advanced Research Center for Nanolithography, Amsterdam, NETHERLANDS;  
S. Krylov, Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow, Russia

In this contribution, we combine theory and basic modeling to address the origin of frictional energy dissipation in dry, unlubricated contacts. Our question is simple: how can this dissipation be so effective? Our calculations demonstrate that the natural mechanism of dissipation is the destructive interference between the phonons that are excited by sliding motion. In the case of stick-slip motion, the energy loss in each microscopic slip event between the sliding bodies readily follows from the dephasing of phonons that are generated in the slip process. The dephasing mechanism directly links the typical timescales of the lattice vibrations with those of the experienced energy 'dissipation' and manifests itself as if the slip-induced motion were close to critically damped. With this, we introduce a new look on sliding friction that may lead to new strategies to manipulate it.

Thursday, November 12, 2020

**9 – 9:55 am - Keynote Presentation**

Patricia Iglesias Victoria, Rochester Institute of Technology, New York

***Protic Ionic Liquids: Economical and Low-Toxicity Lubricants and Additives***

7A

Virtual Breakout Room 1

**Materials Tribology II**

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**Session Chair:** Gustavo Molina, Georgia Southern University, Statesboro, GA

**10 - 10:40 am**

**3435645: "SPOTLIGHT" - Linking Energy Loss in Soft Adhesion to Surface Roughness**

Tevis Jacobs, Abhijeet Gujrati, Subarna Khanal, University of Pittsburgh, Pittsburgh, PA, Siddhesh Dalvi, Ali Dhinojwala, University of Akron, Akron, OH, Lars Pastewka, University of Freiburg, Freiburg, Germany

A mechanistic understanding of adhesion in soft materials is critical in transportation, biomaterials, and soft robotics. On rough surfaces, the apparent work of adhesion coming into contact is lower than the intrinsic value for the materials, and there is adhesion hysteresis during separation. Still lacking is a quantitative experimentally validated link between adhesion and surface topography. Here, we used in situ measurements of contact size to investigate the adhesion behavior of soft elastic hemispheres on four different nanodiamond substrates with topography characterized down to the Ångström-scale. The results show that the reduction in apparent work of adhesion is equal to the energy required to achieve conformal contact. Further, the energy loss during contact is equal to the product of intrinsic work of adhesion and true contact area. These findings reveal the mechanism that links adhesion hysteresis to roughness, rather than viscoelastic dissipation.

**10:40 - 11 am**

**3439418: Tribological Performance of Bearing Bushes Made of Lightweight Mg Matrix Composites**

Juanjuan Zhu, Rob Dwyer-Joyce, The University of Sheffield, Sheffield, United Kingdom

Lightweight metal matrix composites (MMC) are becoming more popular for high efficiency applications, including automobile, aerospace and telecommunication industries. SiC and WS<sub>2</sub> particle reinforcement will further improve the composite properties by enhancing the mechanical strength and reducing the friction and wear between moving parts. In this study, magnesium matrix composites reinforced with 5 wt% WS<sub>2</sub> and 15-20 wt% SiC particles were powder metallurgy sintered and made into bearing bushes. The tribological performance was studied using a purpose built pin joint test rig. It was found that the mechanical properties of the Mg composites were improved by the SiC reinforcement. Under all testing conditions, the Mg composites exhibited lower friction coefficient due to the predominantly physical action of WS<sub>2</sub>.

**11 - 11:30 am - Meet The Experts**

**11:30 am - 11:50 am**

**3435911: Investigation of Formation Mechanisms of Dark Etching Regions and White Etching Bands in SAE 52100 Steel Bearings**

Mostafa El Laithy, Ling Wang, Terry Harvey, University of Southampton, Southampton, Hampshire, United Kingdom, Bernd Vierneusel, Schaeffler AG & Co., Schweinfurt, Germany

Subsurface microstructural alterations such as dark etching regions (DER) and white etching bands (WEBs) manifest in steel bearings due to rolling contact fatigue. It is reported that alterations initiate as DER followed by WEBs which form at an inclined angle of 30° (LABs) first then at 80° to the surface in the

rolling direction. While a number of hypotheses have been presented in literature suggesting formation mechanisms of these features, there is a lack of sufficient experimental evidence in confirming them. The transition from DER to LAB and to HAB is yet to be fully understood. This study focuses on finding formation mechanisms of DER, LAB and HABs through detailed analysis of these features at different stages of the bearing life, including elemental redistribution, dislocation density, mechanical properties and their micro and nano-structures. This study also aims to establish the links between these microstructural changes and final bearing failures.

**11:50 am - 12:10 pm**

**3435695: Direct Measurement of Adhesion for Noble-Metal Nanoparticles Using In Situ Transmission Electron Microscopy**

Andrew Baker, Sai Vishnubhotla, Sanjana Karpe, Yahui Yang, Goetz Vesper, Tevis Jacobs, University of Pittsburgh, Pittsburgh, PA

Metal nanoparticles, due to their small size, exhibit unique functional properties that enable a variety of technologies ranging from renewable energy, to plasmonic sensing, to solid lubricants. Many applications require that these metal nanoparticles are dispersed on a substrate and adhere robustly throughout the service life of the component. Previously, transmission electron microscopy (TEM) has been used to characterize nanoparticles, while scanning probe microscopy has been used to investigate adhesion and friction forces. Here we use in situ TEM adhesion tests to combine these techniques to investigate the science of nanoparticle adhesive interactions. Adhesion tests were performed with nanonewton-scale resolution, with simultaneous imaging to characterize the size, shape, and crystal structure of the nanoparticles and substrates. Results demonstrate the dependence of adhesion energy on chemistry and structure.

**7B**

Virtual Breakout Room 2

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**Lubricants III**

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**Session Chair:** Filippo Mangolini, The University of Texas at Austin, Austin, TX

**10 - 10:20 am**

**3436109: Concentration and Stability Profiles of Copper-Infused Wire Drawing Fluids**

Charles Nider, Floriane Charpentier, Patrycja Adamska, Pascal Bru, FORMULACTION, Worthington, OH

Lubricants that are involved in various types of metalworking or manufacturing environments will eventually undergo particle concentration changes after time and use in machinery. The oil and lubricant components of such emulsions need to be replenished periodically throughout a process. Having quick and quantitative access to this concentration profile information would be critical for operators to adjust their formulations without losing valuable time and efficiency during this process.

We will show how Multiple Light Scattering can be used to quantify physical destabilization phenomena such as particle size and concentration changes without the need for sample preparation or dilution. This technique allows for facile modification of the mixtures if concentrations change or if impurities incorporate themselves into the formulations. This gives operators essential information into the integrity of their dispersions without the need for excessive or objective testing procedures.

**10:20 - 10:40 am**

**3436118: Mimicking of Internal Engine Oil Viscosity at Real Temperature and Shear by Way of a Microfluidic Rheometer**

Charles Nider, Patrycja Adamska, Floriane Charpentier, Pascal Bru, FORMULACTION, Worthington, OH

The high temperature and shear conditions present in combustion and other types of engines are of importance to mimic in order to predict the performance of engine oils and lubricants. Shear-thinning

profiles of oils at these conditions are often extrapolated or estimated when devices of lower acquisition parameters are used while large volumes and longer times are needed with devices operating at higher temperatures and shear ranges.

A novel microfluidic rheometer can fulfill the purpose of mimicking the internal temperature and shear of an engine to provide resolved viscosity profiles of lubricant formulations in a matter of minutes with only several milliliters of sample. This technology eliminates the need for calibration or geometry setup and viscosity is monitored in real-time by visual flow acquisition methods, allowing for high throughput screening in a fraction of time of normal methods.

**10:40 - 11 am**

**3429117: A Novel Approach in the Oil and Gas Industry to Use Tribology Science for the Engineering Design and Evaluation of a Solid Lubricant to Improve Lubricity in Extended Reach Horizontal Wells**

Mario Ramirez, Chevron Phillips Chemical Co, The Woodlands, TX

Contrary to the historically defined evaluative methods in upstream oil and gas, the science of Tribology has not been widely adopted and only a few relevant references can be found in technical industry literature. The coefficient of friction (COF) is considered as a single value used to calculate torque and drag models. Lab equipment used to evaluate the COF does not accurately resemble the conditions of drilling a well.

Extended reach drilling (ERD) generates longer lateral lengths while concurrently pushing the effective limits of oil-based mud and liquid lubricants. A novel solid-state lubricant was developed to reduce friction and extend lateral drilling distances by overcoming the performance limitations of liquid lubricants in extended reach sections.

Development and evaluation of the solid-state lubricant includes the testing of drilling fluids using old and new equipment (Tribometer), highlighting the limitations of traditional upstream lab equipment used to predict the COF. Research also includes the results of field trials in the Permian Basin where the benefits of the solid lubricants have been verified. Well data sets of the torque reading during rotating conditions resemble the Stribeck curves and validate the lab results. The authors believe that this approach contributes to a better understanding of the friction factors in horizontal well development.

**11 - 11:30 am - Meet The Experts**

**11:30 am - 12:10 pm**

**3436105: "SPOTLIGHT" - Optimization of Bio-Derived Basefluid Properties to Improve Efficiency in Hydraulic Systems**

Maria Cinta Lorenzo Martin, Oyelayo Ajayi, George Fenske, Argonne National Laboratory, Argonne, IL, Girma Biresaw, Grigor Bantchev, Roger HarryoKuru, USDA, Peoria, IL

Demand for high efficiency environmentally friendly hydraulic fluids is increasing for a variety of applications, such as agricultural and marine applications. Efficiency of fluid power systems depend on several properties of the hydraulic fluid. The main ones are viscosity (including VI), traction coefficient, bulk modulus, and the boundary friction with appropriate pump and motor materials. Optimization of these properties can provide opportunity for development of efficient hydraulic fluid. Composite fluids consisting of a mixture of PAO and bio-derived ester from high oleic sunflower oil were formulated to have properties similar to commercially available hydraulic fluids. Measurement of the pertinent properties and evaluation of tribological performance indicated the composite fluid has superior or equivalent performance as the current state-of-the-art hydraulic fluids. There are opportunities for further performance enhancement of the composite fluids through formulation.

**12:10 - 12:30 pm**

**3435799: A Molecular Dynamics Approach to Predict Pour Points of Fluids**

Jannat Ahmed, Jie Lu, Q. Wang, Northwestern University, Evanston, IL, Junqin Shi, Northwestern Polytechnical University, Xian, China, Ning Ren, Fran Lockwood, Valvoline Inc, Lexington, KY

Pour point, or the temperature below which a fluid ceases to flow, is an important lubricant property. A molecular dynamics-based approach is used to explore and identify the pour points of a number of fluids. Diffusion properties are investigated at a varying range of temperature and a change in trend around the pour points is observed. A correlation of Solvent Accessible Surface Area (SASA), which is defined as the locus of the center of the solvent probe when it rolls over the molecular surface, and pour point is established. The pour points obtained from the MD simulations are compared with experimental results from literature, and good agreements are observed.

Keywords: Pour Point, Diffusion Properties, Solvent Accessible Surface Area

### 12:30 – 1 pm - STLE Connect- (Exhibits & Posters)

#### 1 – 1:55 pm - Keynote Presentation

David Burris, PhD, University of Delaware

***Cartilage Tribology and the Biomechanics of Joint Health***

7C

Virtual Breakout Room 3

### Machine Elements & Systems I

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**Session Chair:** Robert Erck, Argonne National Laboratory, Lemont, IL

#### 10 - 10:20 am

#### **3418681: The Influence of Oil Film Thickness and Surface Roughness on the Acoustic Emission from Mixed Lubrication Contacts**

Simon Hutt, Alastair Clarke, Rhys Pullin, Pwt Evans, Cardiff University, Cardiff, United Kingdom

Acoustic Emission (AE) refers to the elastic waves that naturally occur in solid materials and are released from a region when it undergoes structural change, for example, when a crack grows. AE has been observed in gears and is typically attributed to the surface asperity interactions that occur in mixed lubrication. In this work, a disk rig was used to generate gear-like EHL contacts and investigate how changes to the lubrication regime affected the AE. Unlike other similar studies, the amount / severity of asperity interactions was independently verified using an electrical resistance measurement technique, and changes to the surface roughness were tracked using in-situ profilometry. A consistent and precise relationship was identified between the AE amplitude and  $\Lambda$  ratio (ratio of oil film thickness to surface roughness). This presentation demonstrates the potential of using AE techniques as a sensitive tool for lubrication monitoring and tribological investigations.

#### 10:20 - 10:40 am

#### **3405390: Wear Effects of Alumina-Nanofluids on Aluminum, Copper and Stainless-Steel Surfaces**

Gustavo Molina, Fnu Aktaruzzaman, Hayden Ohmer, Valentin Soloiu, Mosfequr Rahman, Georgia Southern University, Statesboro, GA

Nanofluids are suspensions of nano-size powders in ordinary fluids and they are intended for use in typical heat-exchangers because of their enhanced-cooling properties. Previous testing by the authors showed that surface modifications (i.e., possible erosion-corrosion effects) occurred from distilled-water-base alumina-nanofluid interactions with aluminum and copper alloy specimens; long-duration jet-impingement tests in a new ad-hoc test-rig yielded substantial roughness modifications, and optical-microscopy showed modified surface features for those typical heat-exchanger materials. Research is presented on similar testing for stainless-steel surfaces which shows, however, no evidence of wear or erosion by the nanofluid on this material, as assessed by the same evaluation methods and for same test-time intervals. The results suggest that the relative hardness of nanopowders, as compared to that of the impacted surface, is an important factor on wear or erosion by the corresponding nanofluids.



**10:40 - 11 am - Open Slot**

**11 - 11:30 am - Meet The Experts**

**11:30 am - 12:10 pm**

**3473456: "SPOTLIGHT" - Use of Tribology in Rolling Bearing Design for Use in Advanced Machinery**

Michael Kotzalas, The Timken Company, North Canton, OH

When people think of the cutting edge of machine design, they often are thinking about electric vehicles, renewable energy or commercial space flight. The last decade has brought about the the beginnings of revolutionary changes in these markets with plug in electric cars or all electric last mile delivery, massive offshore wind turbines, and satellite constellations for global internet and communications coverage. These systems, or the end products that everyone sees, are extraordinary and eye catching, but the design process behind making them work is also highly involved and elegant for those who are knowledgeable in these fields. For the bearing engineer, we must consider new ways of looking at the problems and using tribological theories which allow for the advancements that make these machines work, such as thermal modeling, advanced rheological properties of the fluids, wear testing and material science. Through use of examples, I will discuss how we are implementing these methods into the rolling bearings used in these machines.

**12:10 - 12:30 pm - Open Slot**

**8A**

**Virtual Breakout Room 1**

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**Materials Tribology III**

**Session Chair:** Diane Berman, University of North Texas, Denton, TX

**2:00 pm - 2:20 pm - CANCELLED**

**3435936: In-Situ Observation of Friction and Wear Characteristics of Aluminum Alloys**

Kazuyuki Yagi, Yuya Abe, Joichi Sugimura, Kyushu University, Fukuoka, Japan

Aluminum alloys are used for piston skirt systems and conrod bearings in combustion engines. Although friction and wear behaviors are different from steel, research on friction and wear behaviors of aluminum alloys is little compared with that of steel. In the current study, friction and wear tests of aluminium alloys were conducted using in-situ observation system. A contact area was created between a rotating sapphire disc and an aluminum alloy pin with a curvature. Full formulated engine oil of 0W-8 with MoDTC and ZDDP was used. The contact area was observed over the sapphire disk by a high-speed camera. Three kinds of aluminum alloys were used, which were Al-Si alloy, Al-Sn alloy and Al-Mg alloy to investigate the influence of elements in the alloys on friction and wear characteristics. Chemical reaction film on the alloys was also investigated by SEM and EDS after tests. Friction and wear behaviors with different alloys were compared and discussed.

**2:20 - 2:40 pm**

**3436191: PDA/PTFE + Graphite Particles Coating on 60NiTi: Effect of Coating Thickness and Substrate Roughness**

Dipankar Choudhury, Min Zou, University of Arkansas, Fayetteville, AR

Polydopamine (PDA)/polytetrafluoroethylene (PTFE) + graphite particles (GrP) thin-film coated 60NiTi shows a significantly reduced coefficient of friction and extended wear life in dry contact. In this study, the coating wear life was investigated by changing the coating thickness and substrate roughness. Durability tests were conducted using a linear reciprocating motion at 2, 5, and 10 N applied normal loads against

Si<sub>3</sub>N<sub>4</sub> balls of 6.35 mm diameter. Increasing the coating thickness to 10-13 μm enabled PDA/PTFE+0.25 wt% GrP coatings to continue lubricating 60NiTi through 123K rubbing cycles under 2 N normal load. The coating wear life was further boosted to 150K rubbing cycles by creating a substrate with an average roughness of about 200 nm. However, the wear life of the coating declined to 13K cycles and 5k cycles under 5 N and 10 N, respectively.

**2:40 - 3 pm**

**3436002: The Effects of Incorporating Cu-SiO<sub>2</sub> Nanoparticles in PTFE Top Layer of PDA/PTFE Thin Films.**

Firuze Soltani, Deborah Okyere, Jingyi Chen, Charles Miller, Sujan Ghosh, Mahyar Afshar Mohajer, Nathan Harris, Min Zou, University of Arkansas, Fayetteville, AR

In this study, hybrid Cu-SiO<sub>2</sub> core-shell nanoparticles (NPs) were added to the polytetrafluoroethylene (PTFE) top layer of polydopamine (PDA)/PTFE thin films in order to improve the durability of the films. Three different weight percentage of Cu-SiO<sub>2</sub> nanoparticles (0.005 wt%, 0.0075 wt%, 0.01 wt%) were added to the PTFE dispersion, which was then used to dip coat the PTFE + Cu-SiO<sub>2</sub> NPs on PDA coated stainless steel substrate to form PDA/PTFE + Cu-SiO<sub>2</sub> NP thin films. The resulting thin films had a smaller surface roughness and film thickness compared to PDA/PTFE thin films, demonstrating the effect of Cu-SiO<sub>2</sub> nanoparticles in making compact and interconnected thin films. The more compact films led to improved adhesion, wear resistance, and durability of the PDA/PTFE + Cu-SiO<sub>2</sub> NP thin films.

**3 - 3:20 pm - Open Slot**

**3:20 - 4 pm - Meet The Experts**

8B

Virtual Breakout Room 2

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**Lubricants IV**

**Session Chair:** Demófilo Maldonado Cortés, Universidad de Monterrey, Monterrey, Mexico

**2 - 2:20 pm**

**3439722: Tribological Investigation of Nano-Talc as Additive in Oil Nanolubricants**

Vinay Saini, Jayashree Bijwe, Indian institute of technology, Delhi, Hauz Khas, Delhi, India

Nano-particles (NPs) have been of interest since its inception, due to their extremely small size and large surface area leading to the enhanced surface interaction Nano-lubricants (NLs) or nano-oils are referred to as oils in which NPs are added as an additive in suspension form [1]

This present work aims to explore the investigate the tribological and physical performance of NPs of Talc as an additive in oil that has not been addressed explicitly. The flakes of talc of thickness less than 100 nm were selected for the investigations. The Nano-oils of various (0.5- 4) wt.% concentration of talc particles were formulated using Group III base oils. The oils were characterized for their stability (Visual), density, viscosity and viscosity index and then tribo- investigated on a four-ball tester for anti-wear (AW) according to ASTM D4172 at loading condition of 392, 588 N and EP (weld load) as per IP 239 test standard. An ↑ in Weld load upto 122 % was observed in case of EP performance

Furthermore, to understand the working mechanisms of these nano-oils detailed worn surfaces analysis (Raman spectroscopy, XPS, EDAX, SEM and 3D profilometer) of the balls will be carried out to investigate the nature and type of tribofilm formed. Tribo-sintered talc particles were observed on worn surfaces of in Raman spectra, suggesting the formation of complex tribofilm enriched in C, O and Si elements.

**2:20 - 2:40 pm**

**3440498: Synergistic Effect of Combining TiO<sub>2</sub> and Montmorillonite Clay Nanoparticles as Lubricant Additives for Milling Processes**

Laura Pena-Paras, Martha Rodríguez, University of Monterrey, San Pedro, Nuevo Leon, Mexico, Demófilo Cortés, Gerardo Elizondo, Claudia Rico, Marcela Guajardo, Universidad de Monterrey, San Pedro Garza Garc, NL, Mexico

In this work, nanoparticles of TiO<sub>2</sub> and montmorillonite clay were mixed with varying proportions and added to a cutting fluid for milling of an AISI 4340 steel. Due to its semi-spherical shape and small size nano TiO<sub>2</sub> fill surface valleys reducing friction; montmorillonite, being a multilayer flake-like nanomaterial may reduce friction and wear through exfoliation of their weakly-bonded layers. Laboratory experiments were performed in a four-ball tribotester to determine the best proportions of TiO<sub>2</sub> and montmorillonite clay that provided a synergistic effect. Milling experiments were performed in a CNC equipment with varying feed rate, depth of cut and cutting speed. Plates of AISI 4340 steel were milled with cutting inserts of cemented carbides. A Box Behnken experimental design was performed in order to optimized the milling input parameters and nanoparticle combinations that provided the lowest surface roughness of steel plates, spindle load and wear of cutting inserts.

**2:40 - 3 pm**

**3440344: Interfacial Structure of Adsorption Layer Formed by Polymer-Type Friction Modifier under Temperature Change and Its Nanotribological Property**

Naoki Yamashita, Tomoko Hirayama, Kyoto University, Kyoto, Japan, Honami Watanabe, Ko Onodera, Takehisa Sato, EMG Lubricants Godo Kaisha, Kawasaki, Kanagawa, Japan

We evaluated structural information and tribological characteristics of the adsorption layer of a polymer type friction modifier, which has a methacrylate backbone and hydroxyl groups, formed on a copper surface by neutron reflectivity measurement and frictional tests by an atomic force microscope using the colloidal probe cantilever, respectively. Each experiment was performed under 23 °C and 100 °C to investigate temperature dependence of the adsorption-layer-structure and its nanotribological property. The polymer FM used in this study rapidly approached to a copper surface and then formed about 6-nm-thick adsorbed layer, and the film thickness was about three times larger in 100 °C compared to that in 23 °C. The swollen polymer FM adsorption layer at 100 °C exhibited high load-bearing performance and low friction property. When cooled after heating at 100 °C, the adsorption layer interestingly maintained a swollen state and still exhibited low friction compared to the state before heating.

**3 - 3:20 pm**

**3440430: Structural Analysis of Viscosity Index Improvers in Lubricating Oil by X-ray and Neutron Small-Angle Scatterings**

Tomoko Hirayama, Nobuhiro Sato, Masaaki Sugiyama, Kyoto University, Kyoto, Japan, Ryohei Takahashi, Doshisha University, Kyotanabe, Japan, Yoriyuki Takashima, Kazushi Tamura, Idemitsu Kosan Co., Ltd., Ichihara, Japan, Shinichi Takata, Japan Atomic Energy Agency, Tokai, Japan

Viscosity index improvers (VIIs) are the typical additives in lubricant that work to suppress the viscosity decrease of lubricant against the temperature rise. Classical textbooks say that VII molecules expand their polymer chains in lubricant due to change in solubility in accordance with temperature when the temperature rise, but there are only few papers estimating the 'actual' diameters of VII molecules in lubricant in each temperature. On the background with the recent trend in usage of low viscosity oil, we tried to estimate the actual diameters of VII molecules in lubricant by small-angle X-ray/neutron scatterings (SAXS/SANS). The scattering profiles acquired changing the temperature from 25 to 100C showed that the diameter of VII molecules gradually increased in accordance with the temperature rise, but the behaviour of structural change depended on the chemical structure of VII molecule.

**3:20 - 4 pm - Meet The Experts**

**Machine Elements & Systems II**

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**Session Chair:** Benjamin Gould, Argonne National Laboratory, Lemont, IL

**2 - 2:20 pm**

**3437098: Three-Dimensional Multiphase Physics-Based Model to Study Engine Cylinder-Kit Assembly Tribology**

Sadiyah Sabah Chowdhury, Michigan State University, East Lansing, MI

Controlling wear and emission is pivotal to the improved durability, reduced oil consumption and improved efficiency of the internal combustion engine. The transport of fluids in the cylinder-kit assembly controls friction, wear, oil consumption; influences engine efficiency and emission. This work addresses the understanding of the fundamental aspects of oil transport and combustion gas flow in cylinder kit using simulation tools and high-performance computing. A dynamic three-dimensional multiphase, multicomponent model is demonstrated to study cylinder-kit assembly tribology during the four-stroke cycle of IC engine. The contribution of oil evaporation, oil entrained in the blowby and blowback gas flow for a small-bore engine is investigated. The effect of ring twist on mass flow rate and pressure across the piston is also quantified. The velocity field shows substantial circumferential flow in the piston ring pack leading to high-velocity blowback into the combustion chamber during expansion.

**2:20 - 2:40 pm**

**3439449: Tribological Aspects of Utilizing Wet Friction Materials in Wet Clutch Systems Like Torque Converter Clutches**

Vladimir Klotchikhine, Greening Inc., Detroit, MI

Wet friction materials (WFM) have various application in wet clutch systems like a torque converter clutch (TCC) that is used widely in automatic transmissions, DCT and CVT mechanisms. TCC is a tribological connection with sliding friction contact and boundary and hydrodynamic regimes of lubrication. In TCC, wet friction materials interact with automatic transmission fluid (ATF) and counterface material creating so-called three-elements tribological model. As a member of such friction triangle model WFM play important role: they should provide steady and high friction during engagements, operate smoothly at shifting, mitigate shudder phenomena, resist to ATF fast degradation, and reduce wear of contacting surface. One of the tribological complications in WFM performance evaluation is their variety due to different manufacturing methods. Proposed WFM Technological Identity Group classification allow standardizing materials that help better understand their wear mechanism nature and. Created new tribological model includes five critical elements instead of three typically used helps deeper study their friction performance. Designed criteria help evaluate new TCC on the draft project stage already or estimate existing TCC mechanisms design performance.

**2:40 - 3 pm**

**3440619: Loss Analysis of Radial Magnetic Bearing Using Genetic Algorithm and Gradient Based Method**

Santosh Shelke, Sir Visvesvaraya Institute of Technology Nashik, Nashik, Maharashtra, India

Total loss analysis of four pole pair radial magnetic bearing was performed using genetic algorithm and reduced gradient method. Initially objective functions have been considered, namely minimization total power loss considering three variables like air gap length, rotor speed, and lamination thickness of rotor. Optimum values of these variables and objective function are considered as initial iteration in reduced gradient based method. The implemented method shows genetic algorithm parameters and optimized results are validated.

**3 - 3:20 pm - Open Slot**

**3:20 - 4 pm - Meet The Experts**

**9 – 9:55 am - Keynote Presentation:**

Izabela Szlufarska, PhD, University of Wisconsin-Madison

***Microstructural and Chemical Evolution of Frictional Contacts***

9A

Virtual Breakout Room 1

**Biotribology I**

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**Session Chair:** James Ewen, Imperial College of London, London

**10:00 am - 10:20 am**

**3393437: Innovations in High Performance, Environmentally Acceptable Lubricants (EALs); A Special Focus on Oxidative Stability and Hydrolytic Stability**

Mark Miller, Debby Neubauer, Biosynthetic Technologies, Indianapolis, IN

Green initiatives are everywhere. Bio-fuels, wind energy, renewable fibers are just a few of the environmental initiatives that have recently made headlines. Meanwhile some of the greatest innovations have been in the development and utilization of high performance, environmentally acceptable lubricants (EALs). This paper/presentation focuses on the innovations, features, benefits, strengths and limitation of the different types of EALs. It explores classification of base fluids and additives as well as the requirements of finished lubricants. It compares the performance of conventional petroleum products and biolubricants. The different definitions of environmental acceptability why that is important will be explored. Estolides are a distinct class of esters that has demonstrated exceptional hydrolytic and oxidative stability compared to traditional esters. A modified hydrolytic stability test was developed by Biosynthetic Technologies to monitor the extensive stability of estolides versus traditional lubricant esters over a long duration of time under real world applications.

**10:20 - 11 am**

**3438863: "SPOTLIGHT" - Tribological and Bactericidal Effect of Nanodiamonds as Potential Lubricants for Artificial Joints**

Diana Berman, University of North Texas, Denton, TX

The artificial joints in forms of knee and hip implants are widely used for the treatment of degenerative joint diseases and trauma. Current clinically-used implants, traditionally made from polymer-on-metal structures, often suffer from high friction and wear, leading to associated inflammation and infection resulting in ultimate failure of the artificial joints. Here, we propose an alternative solution to this tribologically-induced failure of the joint materials. We demonstrate that friction and wear behavior of ultra-high-molecular-weight polyethylene (UHMWPE) and titanium tribopair, used to mimic the artificial joint interface, can be improved by introducing nanodiamond (ND) particles in the sliding contact. Analysis of the wear track formed during sliding indicates the formation of a carbon-rich tribolayer of embedded NDs which improves tribological properties of the contacting surfaces and significantly suppressed the wear of the UHMWPE surface. In addition to the improved lubrication characteristics, NDs exhibit high biocompatibility with the bone cells and promising antibacterial properties against *S. aureus*, the most common strain associated with artificial joint infection. These results indicate that NDs can be used as a promising nontoxic human-body lubricant with anti-wear and antibacterial features, thus demonstrating their great potential to treat artificial joint complications through intra-articular injection.

**11 - 11:30 am - Meet The Experts**

**11:30 - 11:50 am**

**3436194: Biotribological Investigation of Cartilage Inspired Textured Ti-6Al-4V and PEEK Interface**  
Dipankar Choudhury, Min Zou, University of Arkansas, Fayetteville, AR

Star-, square-, triangular- and circular-shaped micro dimple arrays were fabricated on Ti-6Al-4V ELI substrates inspired by the porous cartilage topography. Biotribological experiments were conducted on the textured samples against polyether ether ketone (PEEK) pins under in-vitro conditions. It was found that the star-, square- and triangular-shaped [MZ1] [DC2] micro dimple arrays reduced the coefficient of friction by 8% and eliminated the squeaking noise significantly compared to the non-dimpled sample. Notably, the star-shaped micro dimple arrays yielded a substantial wear reduction in both the Ti-6Al-4V discs and the PEEK pins. Microscopic images revealed a large amount of metallic debris transferred from the non-dimpled Ti-6Al-4V discs and embedded on the counterface pins, which is a potential risk for the human body. On the other hand, only minor scratch marks were identified in the star-shaped micro dimple Ti-6Al-4V substrates and the accompanying pins after 30,000 rubbing cycles.

**11:50 am - 12:10 pm**

**3460061: Mechanical and Tribological Behavior of SU-8 Composite Filled with UHMWPE and Gum Acacia Filler**

Jaswant Hirwani, Sujeet Sinha, IIT Delhi, Delhi, India

SU-8 polymer composite with UHMWPE and gum acacia filler was fabricated. The compression modulus and strength of the SU-8/UHMWPE composite decreased with the addition of UHMWPE filler. Tribological test were conducted under albumin lubrication condition using ball on disc machine. Friction of bulk UHMWPE, UH10 (SU-8+10wt%UHMWPE) and UH25 were found to be 0.21, 0.15 and 0.1, respectively and corresponding specific wear rate were measured as 16, 5.86 and  $6.27 \times 10^{-5}$  mm<sup>3</sup>/Nm, respectively. Cross-sectional scanning electron microscopy (SEM) analysis of composite confirmed the micro- fibrillar structure, which helped to bind UHMWPE particles with SU-8 matrix. Adding 10 wt% of gum acacia to UH25 composite reduced the wear rate by 26.6% which can be attributed to the binding properties of gum acacia. Also, the hydrophilic nature of SU-8 composite (water contact angle,  $\theta_1=66.5^\circ$ ) supports protein mediated lubrication compared to hydrophobic UHMWPE ( $\theta_2=97.2^\circ$ ). Therefore, the biocompatible nature of SU-8 and our findings suggest; SU-8 composites can find application in the field of biotribology.

**12:10 - 12:30 pm**

**3480555: Fragile Interfaces**

Angela Pitenis, Allison Chau, George Degen, Jonathan Chen, University of California, Santa Barbara, Santa Barbara, CA

Energy-dissipation mechanisms abound in nature. In natural sliding systems, interfaces are often characterized as "fragile" or "weak" yet they are uniquely capable of mitigating shear stresses, reducing contact pressures, and sustaining adequate lubrication over a wide range of engineering-like challenges where engineered materials have failed. Efforts to characterize these natural interfaces have been limited by their high water content, low polymer concentration, high sample variability, low sample volume, and tendency to age and degrade. Model materials, such as high water content aqueous gels, offer highly tunable and controllable routes towards understanding complex interfacial phenomena and may serve to bridge microscale structure to macroscale properties, such as friction and adhesion. Ongoing research is dedicated to fully understanding the hierarchical structures of fragile interfaces through advanced characterization techniques.

## Lubricants V

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**Session Chair:** Demófilo Maldonado Cortés, Universidad de Monterrey, Monterrey, Mexico

**10 - 10:20 am**

**3439436: Piston Deposit Control: A Fundamental Mechanistic Study**

Anil Agiral, Lubrizol Corporation, Wickliffe, OH

Preventing piston deposit formation is a critical performance property for engine oils. In the current study, we investigated the complex mechanisms of piston deposit control in the Sequence IIIH engine (ILSAC GF-6). We utilized advanced colloid and surface science and new experimental methods to present a unified approach. We will define the molecular and macromolecular structures of oil insolubles in their natural state with spectroscopy, laser reflectance, light scattering and probe microscopy. We will discuss the electrosteric mechanisms of controlling rate and extent of aggregation and deposition of oil insolubles. Our findings confirm the connection between colloidal stability and deposit control.

**10:20 - 10:40 am**

**3439453: Effects of Filtration on Foaming Performance of Anti-Foam Laden Lubricants**

Vinny Suja, Gerald Fuller, Stanford University, Stanford, CA, Abhishek Kar, Shell Global Solutions US Inc., Houston, TX

Non-aqueous lubricant foams are detrimental to lubricated machinery. Lubricant foaming is usually controlled through the use of additives called as antifoams. The size and concentration of these additives are crucial to maintain a satisfactory foaming performance in the lubricant. Unfortunately, the unavoidable filtration of lubricants causes unpredictable variations in the size and concentration of these additives, often resulting in unexpected and adverse foaming performance. Here we study this phenomenon by probing the coalescence stability of single bubbles in filtered lubricants with antifoams. We show that lubricant foam stability is directly correlated to the filtration cycles, and inversely correlated to both the filter pore size and the antifoam concentration. In addition, we also propose a method utilizing single bubble stability to gain an approximate understanding of the underlying antifoam size density distributions.

**10:40 - 11 am**

**3441831: Emission and Vehicle Performance Evaluation of Aged Gasoline Particle Filter via Accelerated Ash and Soot Loading**

Weizi Li, Shell (Shanghai) Technology Limited., Shanghai, China, Yansong Lin, Jinchong Pan, Suzhou Automotive Research Institute, Tsinghua University, Suzhou, China, Chen Yang, Haijun Yang, Geely Powertrain Research Institute, Ningbo, China

To meet recent legislation requirement, gasoline particle filter (GPF) is becoming popular to reduce particle number emission. Ash from engine oil could be loaded on GPF during driving and could potentially impact vehicle performance in long term. In this study, accelerated ash and soot loading methodology through lubricant and fuel mixed combustion for 200k km mileage equivalent is utilized and 3 engine oils with different ash levels or detergent elements were chosen for testing, afterwards WLTC emission, real driving emission, back pressure and engine performance are all measured with loaded GPF. Data shows ash could help particle reduction but has negative impact on gaseous emissions, no significant differences are found between high ash (1.2%) oil and middle ash (0.8%) oil, and either fuel consumption or vehicle power output is not strongly correlated with ash content. But from soot monitoring perspective, we got a motivation to control ash to mitigate the interference.

**11 - 11:30 am - Meet The Experts**



**11:30 - 11:50 am**

**3471418: Grease Behavior in Rolling/Sliding Contacts – On the Neglected Thickener Effects**

Balasubramaniam Vengudusamy, Reiner Spallek, Klüber Lubrication München SE & Co. KG, Munich, Germany

The lubricating film formation and friction behaviors of greases in comparison to oils have been much less reported. Unlike oils, greases are reported to form a very thick film at low speeds, which has commonly been attributed to their thickeners. This could potentially influence lambda ratio, although not many have considered investigating this in detail until recently. Another less explored area is the friction properties of greases. For instance, friction curves (Stribeck curves) of oils are well known whereas those of greases are not reported much. The thick film formation at low speeds could potentially influence the friction, hence the shape of friction curves and lubrication condition of greases might differ from those widely reported for oils. The gaps could be associated with the complex nature of greases. This talk will highlight some key influences of thickener types, base oil viscosity and NLGI grade on film thickness and friction properties.

**11:50 am - 12:10 pm**

**3480054: Tribology of Hydrophilic Polymer Brush Grafted Colloidal Additives in Rolling-Sliding Soft Contacts**

Amir Beheshti, The University of Queensland, Brisbane, Queensland, Australia

Tailoring surfaces by means of concentrated polymer brushes is a robust tool to control friction and wear, but either damage to the brush layer or difficulties of making polymer layers for large surfaces have limited their real applications. Here we have developed hybrid colloids consisted of concentrated polymer brushes grafted silica particles and demonstrate how dispersions of these hybrid colloids enhances lubrication to prevent wear and lower friction by over two orders of magnitude for viscoelastic tribopairs. By subtly changing the solvent quality, the colloids either physically adsorb to the surface or are deposited as a persistent film via the contact forces in the tribometer. These mechanisms mean that the film of hybrid colloids that form on the surface can be tuned and readily replenished from the lubricant, and provide a new strategy for obtaining super-lubricating surface coatings for both biotribological applications and engineering systems.

**12:30 – 12:45 pm - STLE Connect- (Exhibits & Posters)**

**12:45 – 2:00pm - Closing Keynote Presentation:**

John A. Rogers, Northwestern University

***Electronic and Microfluids Systems That Softly Interface to the Skin***

**2 – 2:20 pm - 2020 STLE Tribology Frontiers Week Closing Celebration**

**Graduate Student Poster Session**

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**3468313: Experimental Investigation of Heat Transfer by Internal Flow in Lubrication Film of Non-contact Mechanical Seals**

Yuki Sato, Masayuki Ochiai, Tokai University, Hiratuka, Kanagawa, Japan

Non-contact mechanical seals are used to prevent fluid leaking around the rotating shaft in turbomachineries. On the sealing face of these seals, the fluid lubrication film, which is formed by surface textures, is thin about a few micrometers. Therefore, these seals have excellent performances such as low leakage, low friction torque, and the ability to be used under high-speed and high-pressure conditions. On the other hand, damage by thermal deformation or thermal stress is managed cautiously, because the thin lubrication film is vulnerable to heats. Though the previous studies are discussed that the internal flow affects the film temperature, the flow has not been observed. In this study, the temperature measurements and the visualizations of the flow showed that the temperature is basically higher in the downstream of the flow. In addition, these experiments also show that the temperature distribution is homogenized on the texture with a larger radial velocity component.

**3481958: Tribological Characterization of Gradient-Density Polyacrylamide Hydrogel Surfaces**

Christopher Johnson, Alison Dunn, University of Illinois at Urbana-Champaign, Urbana, IL

The contact and frictional response of hydrogels are dependent on the structure at their surface. Recent work showed that different mold materials used during polymerization will affect the resulting polymer density. We conducted indentation, creep, and sliding experiments with various loads, speeds, and probe materials to determine the impact of the less-dense layer on the contact and frictional behavior of polyacrylamide hydrogels. We used micro-fluorescent particle exclusion to measure the contact areas in-situ. Indentation revealed a non-Hertzian regime for the first 13-29  $\mu\text{m}$  after first contact that has a weaker force response. Creep experiments showed that the surface layer relaxes poroelastically even under miniscule contact pressures. Friction was steady, but highly speed-dependent, with faster sliding speeds experiencing lower friction. This suggests that the surface layer is capable of quick water re-uptake when out of contact. This knowledge may prove useful for hydrogel designs requiring ultra-low friction in a dynamic application.

**3481824: Lubrication and Phase Analysis of an Adaptive Coating at Elevated Temperatures**

Alexander Berendt, Asghar Shirani, Samir Aouadi, Diana Berman, Andrey Voevodin, University of North Texas, Little Elm, TX, Jon-Erik Mogonye, Army Research Lab, Aberdeen, MD

The Army is investigating aviation combustion engine operation leading to major aluminum component temperatures above 300C to increase their efficiency, which has the potential to accelerate wear on the cylinder. Developing a lubricious coating that can reduce wear and function at elevated temperatures will aid in a more reliable engine for aviation operation. This study focuses on a BN/MoS<sub>2</sub>/Sb<sub>2</sub>O<sub>3</sub> 'Chameleon' coating which is designed to have a continuous response to the contact surface in order to provide lubrication [1]. Efforts were made to study the lubricious coating through wear testing with a Nanovea tribometer and Si<sub>3</sub>N<sub>4</sub> counter body to replicate sliding conditions in a cylinder and gather Coefficient of Friction (COF) data to measure the lubricity of this coating during sliding and temperature cycling. Along with the tribometer, an in-situ Renishaw Raman was used to gather real time phase detection at elevated temperatures for analysis of COF data. Further analysis was done on the wear tracks and consequent transfer film present on the counter body by Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS) to view morphological differences and perform elemental analysis. With SEM and EDS, images of a potential transfer film have been gathered and mass transfer onto the counter body is confirmed. Analysis of COF and Raman data also suggests that failure begins when operating temperature rises above 500C and MoS<sub>2</sub> oxidizes.

### **3481782: Lubrication and Phase Evolution of WS<sub>2</sub>/BN/Sb<sub>2</sub>O<sub>3</sub> Chameleon Coatings at Elevated Temperatures**

Euan Cairns, Andrey Voevodin, Samir Aouadi, University of North Texas, Denton, TX, Jon-Erik Mogonye, U.S. CCDC Army Research Laboratory, Adelphi, MD

The increasing use of lightweight alloys in combustion engines demands new surface coatings which protect the metallic substrate from both temperature and wear. In this work, a novel duplex coating architecture consisting of a surface burnished WS<sub>2</sub>/BN/Sb<sub>2</sub>O<sub>3</sub> chameleon coating from pure powder blends, for thermally adaptive lubricity, was applied atop a thermally sprayed yttria-stabilized zirconia (YSZ) thermal barrier coating. The lubrication performance and surface chemical/phase evolution of the duplex coating architecture was evaluated as a function of temperature using a custom-made in situ Raman spectroscopy system coupled with a high temperature tribometer. Scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and X-ray diffraction were used to characterize the coating's composition and microstructure pre and post tribotesting. The friction coefficient of the chameleon coating remained below ~ 0.20 up to 500C, which was correlated to its chemical stability under these conditions as per the Raman spectroscopy data.

### **3481774: Effect of reinforcing PDA/PTFE coatings with silica nanoparticles**

Adedoyin Abe, Min Zou, University of Arkansas, Fayetteville, AR

Polytetrafluoroethylene (PTFE) is one of the lowest friction solid lubricants. In this study, silica nanoparticle (NP) dispersion was mixed with PTFE dispersion and deposited on stainless steel substrates that were coated with a polydopamine (PDA) underlayer. PDA has been shown to enhance the adhesion of PTFE thin coating to the substrate, while silica NPs can improve the mechanical properties of PTFE. The tribological properties of PDA/PTFE thin coatings with or without incorporating silica NPs in the PTFE layer were investigated in dry contact conditions. Coatings were tested using a tribometer under both 2N and 1N normal loads and at a 30% relative humidity. The samples were annealed and then tested in a ball-on-flat configuration in a reciprocating motion. The durability of the PDA/PTFE+silica coatings was improved compared to PDA/PTFE coatings at an appropriate concentration. The wettability, thickness, surface topography, and friction of the resultant coatings were investigated.

### **3481725: Hydrogel thin film friction**

George Degen, Megan Cavanaugh, Allison Chau, Angela Pitenis, University of California, Santa Barbara, Santa Barbara, CA

Thin gel films coat surfaces throughout the human body and provide lubrication and wear protection. Understanding the mechanical properties of these materials, including friction, is important for biomedical applications such as implants. However, biological gel layers are difficult to study directly. Instead, synthetic hydrogels are often used as model systems, but few studies of hydrogels involve biologically relevant film thicknesses. We present an adaptation of the Surface Forces Apparatus (SFA) technique that enables simultaneous measurements of film thickness, friction, and normal force. Using the SFA, we investigate the influences of sliding speed and water content on the friction of microscale hydrogel films.

### **3481693: Determination of Method for Tribological Experiment on Ultra-Hard Coatings in Low-Viscosity Fuels**

Kelly Jacques, University of North Texas, Burleson, TX, Stephen Berkebile, Nikhil Murthy, Jon-Erik Mogonye, US Army Research Laboratory Vehicle Technology Directorate, Aberdeen, MD, Diana Berman, Thomas Scharf, University of North Texas, Denton, TX, Satish Dixit, Plasma Technology Incorporated, Torrance, CA

In order to expand fuel operation capability of fuel systems to multiple fuels, fuel pump materials must resist scuffing and wear when lubricated with low viscosity, low lubricity hydrocarbons and alcohols under conditions of dynamic fluid pressure and flow. In this work, a high-frequency reciprocating tribometer was used to determine a set of tribological experimental parameters that emulate conditions within a fuel pump system, instigate material scuffing, and yield reliable and repeatable results. The ASTM D6079 standard for evaluating lubricity of diesel fuels by the high-frequency reciprocating rig was used as a

basis for the development of new experimental parameters, of which the grinding lay orientation, temperature, counter body, substrate, contact load, and stroke length were altered. These experimental parameters were used to determine the onset of scuffing and wear of through-hardened 52100 steel substrates and various ultra-hard material coatings, including iron boride and tungsten carbides, possible candidates for steel protection. These materials were lubricated with F-24 (JP-8) and ethanol. Scanning electron microscopy, energy dispersive spectroscopy, white light interferometry, and optical microscopy were used to characterize the extent of wear and corrosion of the materials and counter bodies during the experiments. Overall, it was found that the ultra-hard coatings experience less wear and are more resistant to scuffing at low loads than the 52100 steel.

#### **3481709: Nature-Guided Synthesis of Advanced Bio-Lubricants**

Asghar Shirani, Trevor Romsdahl, Kent Champman, Diana Berman, University of North Texas, Denton, TX

Design and modification of environmentally friendly oil-lubricants extracted from biodegradable resources are highly desirable for many applications. Here, *Orychophragmus violaceus* (Ov) seed oil is found to have excellent lubrication properties, because of the unusual structural properties of the major lipid species triacylglycerol (TAG) estolides. Ov TAG estolides contain two non-hydroxy, glycerol bound fatty acids (FAs) and one dihydroxy FA with an estolide branch. Estolide branch chains due to its length, leading to superior thermal stability and lubrication. Using this concept, nature-guided synthetic estolides of castor oil were created. As predicted, they have shown improved lubrication properties similar to Ov seed oil. Our results demonstrate a structure-based design of novel lubricants inspired by natural materials.

#### **3481678: Tribotronic Design and Control of Metal Oxide Nanofluid Interfaces.**

Caitlin Seed, Biplav Acharya, Alex Smirnov, Jacqueline Krim, North Carolina State University, Raleigh, NC

Interest in metal oxide nanoparticle suspensions is rapidly growing in a wide range of applications owing to their environmental friendliness and ease of mass-production. Focusing on energy storage applications, we report an experimental study of tribotronic control of TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> nanoparticles at Pt-water interfaces. The measurements demonstrate a means to incorporate tribological performance into the design of energy systems. We observe a high degree of correlation between the voltammetry and tribological performance measures, and evidence for pseudocapacitance of NP. The cyclic voltammetry data moreover reveal energy storage levels for NP pressed temporarily in place by electrostatic fields to be comparable in magnitude to those reported in the literature for rigidly attached TiO<sub>2</sub> NP structures.

#### **3481411: Molecular Dynamics Simulation of the Chemical Adsorption of Phosphate Esters on Metal Surfaces**

Mutsuki Homma, University of Hyogo, Kashihara, Nara, Japan

The adsorption behavior of phosphate esters additives which are used as extreme pressure agents in machine oils are analyzed. Molecular dynamics (MD) methods, which can treat dissociation and formation of covalent bonds are used. We analyze the adsorption process by observing the charge transfer and the amount of transfer of the compound. Both Fe and Fe oxidized surfaces are used for metal surfaces. As the additives, 3,5-diethyldodecanes as base oils, and monooleylphosphates or diolelylphosphates as extreme pressure additives are simulated. As a result of the analysis of the surface diffusion and charge transfer, it is confirmed that the adsorption process is physisorption followed by chemisorption.

#### **3481402: Analysis of the Stability of Organophosphate Aggregates in Oil by Molecular Dynamics**

Kyosuke Kawakita, Yoshiki Ishii, Hitoshi Washizu, University of Hyogo, Kobe, Japan, Hiroaki Koshima, Idemitsu Kosan Co.,Ltd., Tokyo, Japan

Oiliness improver and extreme pressure additive are representative of additives for machine oils. Although, the fatty acids and the organophosphate have similar physicochemical structures with alkyl chains attached to polar groups, the tribological usage is very different, i.e. the latter acts in severe

condition such as high temperature and heavy load. In this study, molecular dynamics simulations of material systems are performed using 3,5-diethyldodecanes as base oils, and monooleylphosphates or diolelylphosphates as extreme pressure additives. As reported in our previous study, multiple extreme pressure additive molecules form aggregates within 1 ns in both systems, and it is difficult to reach the charged surface. The mean square displacements of extreme pressure additive and base oil indicate that monooleylphosphate is more diffusive than diolelylphosphate, and the difference in the molecular weight of the extreme pressure additive affects the diffusion coefficient of the base oil.

#### **3481395: Chemical Reactions in Zirconia and Metals Under Friction**

Yosuke Hamano, Hirotooshi Akiyama, Yoshiki Ishii, Hitoshi Washizu, University of Hyogo, Kobe, Hyogo, Japan

The possibility of Frictional Fade-Out (FFO) phenomena is investigated in the friction system between zirconia (ZrO<sub>2</sub>) and metal surface. FFO refers to the phenomenon of a significant decrease in the coefficient of friction between ZrO<sub>2</sub> and Diamond-Like Carbon (DLC) when they are exposed to a special environment (1). The characteristics of the ZrO<sub>2</sub>, which is catalysis of hydrogenation, have a significant influence on the conditions for the phenomena of FFO. Therefore, the same phenomenon as FFO may be confirmed when conditions for FFO are met even if the partner material of ZrO<sub>2</sub> is other than DLC. In this paper we investigate the friction of ZrO<sub>2</sub> in order to consider the possibility of FFO by using molecular dynamics simulations including chemical reactions. Nickel (Ni) was used as the partner material. Ethanol and hydrogen radicals are placed between the ZrO<sub>2</sub> and Ni in order to replicate the environment of the experiment in which the FFO was reported. In the experiment, the ethanol molecules are used to make the transfer layer on the ZrO<sub>2</sub> surface.

#### **3481379: Effect of Water Atmosphere on Friction of Multilayer Graphene Studied by Reactive Molecular Dynamics**

Ryo Matsuoka, Yoshiki Ishii, Hitoshi Washizu, University of Hyogo, Kobe, Japan

MD simulation using reactive force fields revealed the involvement of graphene functional groups in the friction of layered graphene transfer layers. At the hydrogen termination case and in vacuum and in low temperature of 50 K, the thermal escape motion which is found in previous studies is reproduced. In the hydroxyl group termination system in vacuum, the thermal escape motion is inhibited by the functional group. On the other hand, the thermal escape motion is reproduced by surrounding these inhibited systems with a population of water molecules in room temperature. Thus, it is found for the first time that the low friction of graphite is greatly affected by the surrounding water molecules in both hydrogen termination and hydroxyl termination. This is due to the hydrophobic interaction to stabilize the transfer graphene layer.

#### **3481336: Study of Tribological Properties of Laser Micro Texturing under Polyalphaolefin-40 Condition**

Junru Pang, Hong Guo, Patricia Iglesias, Rochester Institute of Technology, Rochester, NY, Juan Manuel Vazquez Martinez, Jorge Salguero, University of Cadiz, Puerto Real, Cadiz, Spain

Laser surface texturing (LST) has gradually become a competitive surface treatment method to fabricate controllable micro-scale structures, which can significantly improve the tribological behavior of the material surface. Compared to untextured surfaces, the friction and wear can be significantly reduced by applying micro-scale textures to sliding surfaces. In this work, the effect of laser textured surfaces on the tribological performance of titanium alloy-Ti6Al4V was studied, where the textured surfaces were prepared by changing the energy density of pulse and distance between dimples. The frictional tests were conducted by using a ball-on-flat reciprocating tribometer under ceramic-Ti6Al4V contact lubricated by Polyalphaolefin-40 (PAO 40). The contact angles of PAO 40 on textured surfaces were examined to be smaller than that on the untextured surface. Compared to the untextured surface, the tribological performances of textured surfaces were significantly enhanced, where the reduction of friction and wear is up to 19 % and 28 % respectively.

### **3473304: Study on High-Speed Friction Behavior of Tread Rubber by Thermo-Mechanical Coupling Method**

Da Chen, Jian Wu, Benlong Su, Fei Teng, Youshan Wang, Harbin Institute of Technology, Weihai, Weihai, Shandong, China

Due to the high landing speed, high-speed friction behavior is important to the safety of aircraft, which generates a lot of heat. Firstly, high speed friction test device has been developed to study high-speed friction behavior, and the temperature was recorded by FLIR E4 infrared thermal imaging camera. Then, the influence of load, velocity on the friction force and temperature have been investigated. Finally, a thermo-mechanical coupling finite element model of friction behavior has been developed, which considered the influence of strain amplitude on the hysteresis lost. Results indicated that the predicted friction forces and temperature were agreement with that of experiment; the effect of radius of pavement particle on the friction temperature was not obvious. The coupling method based on high speed friction test and FEM provides a basis for design and optimization of aircraft tire.

### **3481264: Effects of Test Parameters on the Frictional Properties of Al/a-Si Core-shell Nanostructures**

Colin Phelan, Min Zou, University of Arkansas, Fayetteville, AR

Friction tests are useful in determining whether a material or textured surface displays tribological benefits. However, the parameters of these friction experiments can largely influence the results. In this study, Al/a-Si core-shell nanostructures are tested, with three varying parameters: normal load (10  $\mu\text{N}$ , 100  $\mu\text{N}$ , and 500  $\mu\text{N}$ ), the counterface indenter tip radii (1  $\mu\text{m}$ , 5  $\mu\text{m}$ , and 20  $\mu\text{m}$ ), and tip position during tests. At the lowest normal load tested, the largest tip resulted in the lowest COF values. During the higher load tests, the 5  $\mu\text{m}$  tip generated the lowest COF values. The position of the tip during the experiments had the greatest effect on the measured COF for the smallest tip, while the largest tip was unaffected. This study provides a further understanding of the effects and their significance of each friction test parameter and investigates the mechanisms which control these effects.

### **3481206: Evaluation of Viscosity of Oil Solution with Viscosity Index Improver by Hybrid Simulation**

Gentaro Sawai, Taiki Kawate, Soma Usui, Hitoshi Washizu, University of Hyogo, Kobe, Hyogo, Japan

It is known that engine oil can be made to have a higher VI by adding a viscosity index improver (VII). However, the theoretical equation for predicting the viscosity of base oil by the addition of VII has not been established because the magnitude of the effect of hydrodynamic interactions acting on the VII molecule is unknown. In this study, the behavior of VII is simulated in a microscale analytical space that reproduces the sliding environment of the engine using a hybrid simulation method that combines the lattice Boltzmann method and Brownian dynamics to investigate the magnitude of the effect of dissipative forces acting on the VII molecules. Three shear rates of 1 m/s, 10 m/s and 100 m/s were used in the simulation. As a result, there was no difference in the dissipative force acting on the VII molecule over time at the three shear rates. This suggests that the random force from the base oil has a considerably larger effect on the VII molecule than the mainstream velocity.

### **3481193: Molecular Dynamics Analysis in Long-Chain Molecular Systems of Traction Mechanism**

Ryoichi Katsukawa, Eiji Tomiyama, Hitoshi Washizu, University of Hyogo, Nishinomiya, Hyogo, Japan

Molecular dynamics simulation is used to estimate the traction coefficient for the long chain hydrocarbon lubricants, which is used in machine elements for elevators and so on. In this study, in order to investigate the influence of the structure of fluid molecules in the shear field, the traction simulation is used by adding pressure and movements in confined by solid system, and calculated the traction coefficient in elasto-hydrodynamic condition [1-3]. In order to simulate the traction phenomena in small simulation cell, wider cell size is used to investigate the a steady state. Figure 1 shows a snapshot at constant pressure and constant shear. The average traction coefficient was calculated, and  $\mu = 0.42$ , which is larger than the small fluid molecules. The molecular origin of traction phenomena in long chain molecules is then analyzed in this system.

**3481165: Compositional dependence of polyacrylamide hydrogel abrasive wear resistance**

Shabnam Bonyadi, Alison Dunn, University of Illinois at Urbana-Champaign, Urbana, IL

Hydrogels are polymer networks that retain large volumes of water allowing for low friction sliding. In this work, a sandpaper covered probe attached to a microtribometer with a reciprocating stage was used to wear polyacrylamide hydrogels with varying concentrations of polymer and crosslinker. A 3D Laser Scanning Confocal Microscope was used to analyze the resulting wear scars. Because increasing polymer concentration and crosslinker concentration both increase the stiffness of hydrogels through different structural mechanisms, they affect different aspects of the wear response of the material. We calculated the wear rates for the different compositions and developed a relationship that connects the polymer and crosslinker concentrations to the wear rates. These results suggest that network flexibility and swelling potential strongly influence hydrogel wear behavior. This work is the beginning of developing more accurate predictions of the wear behavior of biphasic materials.

**3481079: Traceable Lateral Force Calibration (TLFC) for Atomic Force Microscopy**

Arnab Bhattacharjee, David Burris, University of Delaware, Newark, DE, Nikolay T. Garabedian, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Calibration of a probe or device beforehand is mandatory to accurately measure applied force during an experiment. Probe of a micro/macro tribometer is usually calibrated with the help of precise weight balance. On the other hand, efforts to reliably measure AFM lateral forces have been impeded by the difficulties in obtaining appropriate calibration standards, applying those force standards to the apex of the tip, and quantifying calibration uncertainty. Here we propose a new method, Traceable Lateral Force Calibration (TLFC), which combines the reliability of direct methods with the convenience of indirect/semidirect methods. This study has revisited the already known reference lever method to come up with a simple and traceable device for lateral force calibration. Calibration of AFM probes (integrated and colloidal) in different AFM instruments (dimension 3100, multimode) and friction measurements on Si-wafer has been presented in this paper.

**3480888: Mechanisms of Graphite Lubrication under High Mechanical Load**

Carina Morstein, Martin Dienwiebel, Karlsruhe Institute of Technology, Karlsruhe, Germany

Carbon-based materials have been employed for decades as solid lubricants for applications where liquid lubricants reach their limits, e.g. under high temperature, in vacuum, or under high mechanical loads. In this study, the fundamental wear mechanisms of graphite were studied in sliding friction under high mechanical load. For these investigations, graphite coatings of various thickness were applied with an airbrush spray gun onto substrates with two roughness levels. In microtribometer experiments an increase of the coefficient of friction due to ploughing was observed at increasing graphite thickness, as well as a decrease in wear and an elongation in lifetime. As the normal load was elevated up to 1 GPa a decrease in friction was observed with a coefficient of friction as low as 0.12. By increasing the substrate roughness, a drastic improvement in terms of friction, wear, and lifetime could be achieved due to the formation of a stable, thin carbon layer in the tribocontact.

**3476397: Nanoscale Solid Lubrication Achieved with  $Ti_3C_2T_x$  Nano-sheets (MXenes)**

Md Shah Jaman, Anthony Rodriguez, Ogulcan Acikgoz, Mehmet Baykara, University of California Merced, Merced, CA, Bo Wang, Jinhong Yu, Ningbo Institute of Material Technology & Engineering, Ningbo, China, Philipp Grützmaier, TU Wien, Vienna, Austria, Andreas Rosenkranz, Universidad de Chile, Santiago, Chile

$Ti_3C_2T_x$  nano-sheets (MXenes) are an emerging class of two-dimensional materials with outstanding potential to be employed in energy storage, catalysis, and triboelectric applications, on length scales ranging from the nano- to macroscopic. Despite rapidly accelerating interest in this new class of materials, their nanoscale frictional properties and in particular, their potential for solid lubrication on the nanoscale, have not been explored in detail yet. Here, we present the first results on the nanoscale frictional characteristics of MXenes, in the form of a friction map obtained on an isolated  $Ti_3C_2T_x$  nano-sheet deposited on a silicon dioxide substrate via friction force microscopy [1]. Our experiments reveal that few-

layer  $Ti_3C_2T_x$  nano-sheets indeed act as solid lubricants on the nanoscale, reducing friction on the silicon dioxide substrates, although not as effectively as few-layer graphene. The results reported here pave the way for further studies focusing on nanoscale solid lubrication achieved by  $Ti_3C_2T_x$  (MXene) nano-sheets. [1] Rodriguez, A., Jaman, M.S., Acikgoz, O., Wang, B., Yu, J., Grutzmacher, P.G., Rosenkranz, A., Baykara, M.Z., The Potential of  $Ti_3C_2T_x$  Nano-sheets (MXenes) for Nanoscale Solid Lubrication Revealed by Friction Force Microscopy, Applied Surface Science, DOI: 10.1016/j.apsusc.2020.147664, (2020).

### **3476936: Mechanical and Tribological Characterization of Sodium Alginate Hydrogels Reinforced with Carbon Nanotori**

Daniel Quintanilla Correa, Juan Moreno González, Laura Pena-Paras, Roman Vidaltamayo, University of Monterrey, San Pedro, Nuevo Leon, Mexico, Oxana Kharissova, Patsy Arqueta, Universidad Autónoma de Nuevo León, San Nicolas de los Garza, Nuevo León, Mexico, Antonio Sánchez-Fernández, Instituto Tecnológico y de Estudios Superiores de Monterrey, Monterrey, Mexico

In this research, alginic acid hydrogels reinforced with different concentrations (0, 0.01, 0.05 and 0.1 wt.%) of carbon nanotori were characterized, acquiring their compression, tension and tribological properties. Tension and compression tests were performed using a multi-test dynamometer adding calcium chloride as a crosslinking agent obtaining solid samples. Extreme pressure tests according to the ITEePIB Polish method were executed using a four-ball T-02U tribometer measuring the performance of non-crosslinked hydrogels as lubricants. In the tensile tests, the non-reinforced hydrogel obtained an Ultimate Tensile Strength (UTS) of 19 MPa, being surpassed by all the reinforced hydrogels, especially by the one reinforced with 0.1 wt.%, with 44.43 MPa. Tribological tests obtained a positive response for the addition of nanoparticles, showing an increment of 105% in the contact limit pressure ( $\rho_{oz}$ ) for the hydrogel reinforced with a 0.05 wt.% compared to the non-reinforced hydrogel. In contrast, the addition of nanotori did not have a noticeable improvement in the compression tests, with only a 3.4% increase in the Ultimate Compressive Strength (UCS) obtained by the hydrogel reinforced with 0.05 wt.% compared with the hydrogel without nanoparticles.

### **3477773: Scratch Study of 60NiTi/PDA/PTFE Coating Using a Diamond Nanoindenter Tip**

Charles Miller, Min Zou, University of Arkansas, Fayetteville, AR

60NiTi exhibits the intriguing combination of low elastic modulus and high hardness. These properties, along with many others, have made this material an interesting candidate for bearing and aerospace applications. In this study, a nanoindenter equipped with a spheroconical diamond tip of 5  $\mu$ m diameter and a scanning electron microscope were used to evaluate the friction and deformation of a polytetrafluoroethylene (PTFE)-based solid lubricant coating with a polydopamine adhesive underlayer on 60NiTi. Scratch normal loads ranging from 25-8000  $\mu$ N were used. The coefficient of friction (COF) showed an interesting behavior with the changing applied normal load. At low loads, the COF was the highest. As the load increased, the COF first decreased and then increased and decreased again. SEM imaging of the scratches helped elucidate the COF behavior in the context of adhesion and deformation mechanisms of friction.

### **3478010: Structure-Property Relationships of Gradient Hydrogels**

Allison Chau, Eric Valois, Angela Pitenis, University of California, Santa Barbara, Santa Barbara, CA

Soft aqueous gels are commonly utilized to model biological materials due to their ability to mimic the mechanical and tribological properties of these soft tissues. Poly(acrylamide) (PAAm) is a highly characterized hydrogel that is often utilized for this purpose because the average spacing between crosslinked chains, the mesh size ( $\zeta$ ), can easily be tuned by controlling polymer and crosslinker concentrations.

This work focuses on the characterization of PAAm hydrogels intentionally fabricated with a gradient in crosslinking density through oxygen-inhibited free radical polymerization to gain fundamental understanding of the interplay between processing, structure, and mechanical property. The elastic moduli and friction coefficients of hydrogels with a gradient ("surface gradient hydrogels") were compared to those with comparatively uniform crosslinking density. A contact mechanics model combining draining and Winkler mechanics was derived to model the mechanics of the surface gradient hydrogel and



compared against typical Hertzian and Winkler contact mechanics.

**3478811: Engineering Hydrogel Surfaces for Controlled Frictional Behavior**

Alex Deptula, Rosa Espinosa-Marzal, University of Illinois at Urbana-Champaign, Urbana, IL

With recent developments in soft robotics, novel stimuli-responsive materials are desired for controlling interfacial forces. Hydrogels have been a topic of interest in biotribology for decades due to their biocompatibility, extremely low coefficients of friction, and compositions similar to that of biotribosystems. The present work focuses on tuning the phase separation of negatively charged poly(acrylamide-co-acrylic acid) hydrogels to achieve controlled frictional responses. The topology of the hydrogels was studied through Quantitative Imaging using an Atomic Force Microscope, which allowed sub-micrometer resolution of stiffness and adhesion variations on the surface of the hydrogels. Phase separation within the gels was modulated by altering the ratio of acrylamide to acrylic acid monomer. This led to concurrent phase and microphase separation within a sample and thereby to topological variations. These topological variations will subsequently change the gel's contact mechanics.

**3480795: Shakedown Analysis of Evolving Non-Hertzian Rolling Contact Using a Semi-Analytical Numerical Model**

Yaswanth Sai Jetti, Alison Dunn, University of Illinois Urbana-Champaign, Urbana, IL

The non-conforming rolling contact under high loads results in considerable plastic deformation of the surface. This surface plastic flow was studied using a twin-disk tribometer, and the observed deformation as a function of the number of rolling cycles was classified into three distinct stages. In the initial stage, the contact type changed from Hertzian to non-Hertzian in the first few cycles and then changed from non-Hertzian back to near Hertzian by the end of this stage. A semi-analytical model, using overlapping hexagonal traction elements, was therefore employed to perform the contact analysis. The contact area was observed to change from elliptic to a near rectangular. Shakedown limits were obtained at different instants of the deformation process using Melan's theorem. The actual stress state was observed to move on a shakedown map until it went below the elastic limit and finally converged to a stress state within the elastic zone.

**3479396: Modelling and Designing the Electrical Contact of Two-Dimensional Interfaces**

Aisheng Song, Ruoyu Shi, Zhiwei Yu, Jianbin Luo, Tianbao Ma, Tsinghua University, Beijing, China, Lei Gao, University of Science and Technology Beijing, Beijing, China

Contacting interfaces with physical isolation and weak interactions usually act as barriers for electrical conduction. Reducing the contact resistance is crucial but a great challenge for designing high-performance microscale and nanoscale functional devices, which call for thoroughly basic theory study and reasonable material design.

In the basic theory study aspect, we establish a relationship between the atomic-scale contact quality (ACQ) and local interfacial atomistic structure. This real-space model unravels the atomic-level spatial modulation of contact conductance, and the twist angle dependent interlayer conductance between misoriented graphene layers.

In the material design aspect, we propose an effective strategy to obtain both low friction and high conductivity in sliding electrical contacts, which provides a potential strategy for tackling the dilemma for high performance sliding electrical contacts.

**3487374: Interfacial Rheology of Hydrogel-like Materials Using an Extended Surface Forces Apparatus (eSFA)**

Tooba Shoaib, Rosa Espinosa-Marzal, University of Illinois at Urbana-Champaign, Urbana, IL

Since their inception, hydrogels have gained popularity among multiple fields, most significantly in biomedical research and industry. Due to their semblance to biological tribosystems, a significant amount of research has been conducted on hydrogels to elucidate biolubrication mechanisms, however, the pathways and mechanisms of the viscous dissipation are still widely debated. Investigating the rheology of thin hydrogel films along with their tribological response and response to compression can enable us to

understand the underlying lubrication mechanisms. We have employed the extended Surface Forces Apparatus (eSFA) in a dynamic shear fashion to quantify and understand the relation between interfacial rheology and underlying lubrication mechanisms of single network hydrogels for the first time. Steady and dynamic shear measurements were performed on hydrogel thin films (~2-6 mm in thickness) under modulated compressions. The amplitude and frequency sweeps reveal a change in the hydrogel's structure and rheological response as a function of compression. These experiments provide new insight into the viscous response of the hydrogel thin films to shear, hence enabling to evaluate, understand and model the frictional response from the perspective of hydrogel's biphasic nature.

**3487720: Ionic Liquid Lubrication Studied Via Nanorheology and Nanotribology**

Mengwei Han, Rosa Espinosa-Marzal, University of Illinois at Urbana Champaign, Urbana, IL

Ionic liquids (ILs) have been recognized as suitable lubricants for harsh conditions and enable electro-tunable lubrication. The strongly adsorbed ILs layers on the solid interface are capable of bearing heavy loads and effectively reduce friction. We study the nano-confined IL layers using a nano rheometer that is developed from an extended surface forces apparatus (SFA). Three ILs are investigated to understand the influence of the ions' chemical structures. The influence of water is studied by equilibrating the ILs at fixed humidity to introduce water from the gas phase. Among the three ILs, the layer (s) closest to the solid interface is found to be elastic, after the upper layers of ions are squeezed out of the confined region. Water is found to alter the viscoelastic behavior of the nanoconfined IL layers. The results from the nanorheological tests are compared to friction measurements with the SFA, as function of both applied load and sliding velocity. Friction varies with sliding velocity in the range of investigated velocities, and severe stick-slip is observed in the regime of slow velocities that correlates with the highest friction. The presence of water alters the tribological response. The work will shed light on the molecular mechanisms that govern IL lubrication.

**3488581: Effect of Roughness on the Friction Characteristics of Single Calcite Crystals**

Binxin Fu, Rosa Espinosa-Marzal, University of Illinois at Urbana-Champaign, Urbana, IL

Fault slip may be promoted by fracture of asperities and intergranular lubrication mediated by water in the fault, among others, and an earthquake could be triggered as a result. Another phenomenon that can lead to the reduction in friction in aqueous environment is so-called pressure solution facilitated slip, where enhanced contact stress leads to dissolution of minerals so the dissolved ions efficiently lubricate the contact. This phenomenon has been confirmed with an idealized model of carbonate rock: smooth calcite cleaved along crystalline plane. On the other hand, it still remains unknown how the results on smooth calcite relate to the real-world situation. Understanding the frictional response at multi-asperity contacts, representing the complex contacts between rocks in nature, could give insight into further mechanisms affecting friction, e.g. asperity interlocking and contact healing. The friction on well-characterized rough calcite shows a logarithmic trend at high sliding velocity as predicted by transition state theory. However, there is deviation from the trend at high stress and low sliding velocity at all investigated roughness, suggesting the friction weakening caused by pressure solution. This indicates that pressure solution slip may be a general phenomenon in rock friction regardless of the contact smoothness. Furthermore, the contact roughness has an important effect on the frictional weakening, which is discussed here in detail.

## Undergraduate Student Poster

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### **3476654: Synergistic Effect of Combining TiO<sub>2</sub> and Montmorillonite Clay Nanoparticles as Lubricant Additives for Milling Processes**

Marcela Guajardo, Claudia Rico, Gerardo Elizondo, Universidad de Monterrey, San Pedro Garza García, Mexico

In this work, nanoparticles of TiO<sub>2</sub> and montmorillonite clay were mixed with varying proportions and added to a cutting fluid for milling of an AISI 4340 steel. Due to its semi-spherical shape and small size nano TiO<sub>2</sub> fill surface valleys reducing friction; montmorillonite, being a multilayer flake-like nanomaterial may reduce friction and wear through exfoliation of their weakly-bonded layers. Laboratory experiments were performed in a four-ball tribotester to determine the best proportions of TiO<sub>2</sub> and montmorillonite clay that provided a synergistic effect. Milling experiments were performed in a CNC equipment with varying feed rate, depth of cut and cutting speed. Plates of AISI 4340 steel were milled with cutting inserts of cemented carbides. A Box Behnken experimental design was performed in order to optimized the milling input parameters and nanoparticle combinations that provided the lowest surface roughness of steel plates, spindle load and wear of cutting inserts.

### **3477993: Tribological Characterization of Vegetable Lubricants Reinforced with Halloysite Clay Nanotubes**

Jose Gonzalez Garcia, Ricardo Duran, Ricardo Cantu Peña, Universidad de Monterrey, Monterrey, Nuevo Leon, Mexico, Laura Pena-Paras, University of Monterrey, San Pedro, Nuevo Leon, Mexico, Demófilo Cortés, Universidad de Monterrey, San Pedro Garza Garc, NL, Mexico, Javier Ortega, University of Texas Rio Grande Valley, Brownsville, TX

Manufacturing processes commonly use lubricants to decrease the friction between moving components, reducing vibration and improving the efficiency of the process. Usually these cutting fluids or lubricants are based on mineral oils and have additives which are not environmentally friendly, increasing the costs of the process from lubricant disposal. Therefore, there is an increasing need to employ environmentally friendly lubricants such as vegetable oils. Nanoparticles additives have also been studied in order to improve the tribological properties of these lubricants. In this study, lubricants of soy, corn, peanut and sunflower seed were additized with environmentally-friendly halloysite clay nanotubes in concentrations of 0.01, 0.05, 0.10 wt.% by ultrasonication. Tribological properties were characterized under anti-wear and extreme-pressure conditions using a T-02 four-ball and a T-05 block-on-ring tribotesters. The results of this study demonstrate the potential of bio based nano-lubricants to be used in manufacturing processes.

### **3480794: Low Cost, Environmentally-Friendly Protic Ionic Liquids as Lubricants and Lubricant Additives**

Brandon Stoyanovich, Patricia Iglesias, Hong Guo, Rochester Institute of Technology, Miami, FL

Much of the world's leading lubricants used are petroleum-based which are harmful to the environment and cannot sustainably biodegrade. Alternative greener options have been found to help replace toxic chemicals altogether. In this study, three ecofriendly protic ionic liquids (PILs), 2-hydroxyethylammonium p-toluenesulfonate (Ets), 2-hydroxymethylammonium p-toluenesulfonate (Mts), and 2-hydroxydimethylammonium p-toluenesulfonate (Dts) were synthesized and tested as lubricant additives. The three PILs were respectively mixed with a base biodegradable oil (BO) with a concentration of 1 wt.%. The wear and frictional performance of the three PIL blends, BO and a commercial biodegradable oil (BOA) were investigated by using a ball-on-flat reciprocating tribometer under aluminum-steel contact. The use of any PIL as additive to BO reduced the friction coefficient compared to BO and BOA. Particularly, an astounding friction decrease of 39.6% was obtained by using 1 wt.% Mts+BO with respect to BO. A 15.9% reduction in wear volume was achieved using 1 wt.% Ets+BO.

### **3481287: Tribological Behavior of Prototyped Polymers**

Alexis Saucedo, Demófilo Cortés, University of Monterrey, San Pedro Garza García, Nuevo León, Mexico, S.N. Mazurchevici, Dumitru Nedelcu, R. I. Popa, C. Carausu, Technical University of Iasi, Iasi, Romania, Laura Pena-Paras, University of Monterrey, San Pedro, Nuevo Leon, Mexico

Now days the world requires new engineering alternatives in order to satisfy the actual ecological and energetic needs. With the present-day technologies combined with innovative engineering and scientific processes, developed new ecological solutions are possible. Humanity has had made big research in the tribology's field to bring humankind new solutions and with that make a change in the way how they live, but it's not enough. New challenges emerge as time goes on and tribologists have to be prepared to deal with them, cooperating with other colleagues and using all available resources. This research use material A compared with other composite material B (manufactured by 3D printing technology) to evaluate their tribological behavior (wear and friction coefficient). The purpose of this scientific exposition is to demonstrate the tribological impact of these polymers on possible industry applications, replacing old conventional plastics with new ones. Also, some of the authors developed researches on the dynamic behavior of 3D printed samples, studied the mechanical and thermal properties, just to make a connection with the tribological properties. As a conclusion it can be stated that the results obtained certainly lead to the possibility of replacing some plastics with the studied biodegradable materials.

## Early Career PhD Poster

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### **3480228: Tribocorrosion of a Nickel-Free High Nitrogen Steel vs. LC-CoCrMo in Simulated Synovial Fluids**

Simona Radice, Alfons Fischer, Markus Wimmer, Rush University Medical Center, Chicago, IL

We have compared the tribocorrosion of the well-established CoCrMo-alloy, with that of a Ni-free high nitrogen steel, in clinically relevant test-fluids, including simulated inflammatory conditions by addition of hydrogen peroxide.

LC-CoCrMo alloy and FeCrMnMoN steel disk-samples were tested in triplicate against a ceramic ball on a custom made tribometer, using a published protocol. Simulated synovial fluids were prepared with: Dulbecco's phosphate buffered saline solution; newborn calf serum; hyaluronic acid; and hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>). Samples wear was quantified through measurements of wear scar volume (OrthoLux, Redlux).

Without H<sub>2</sub>O<sub>2</sub>, wear scar volumes were similar for both metals. However, wear of LC-CoCrMo increased with increasing H<sub>2</sub>O<sub>2</sub>, while this was not the case for FeCrMnMoN.

Our results indicated a favorable tribocorrosion performance of FeCrMnMoN compared to LC-CoCrMo. Further research is needed, to fully understand the mechanisms behind our findings, and to be able to propose the Ni-free FeCrMnMoN for certain biomedical applications.

### **3481025: Liquid-repellent coatings for friction reduction on hydraulic pump components**

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In this study we investigated the role of nanostructured coatings deposited on piston slippers surface aiming at improving their overall efficiency through a significant reduction in fluid friction losses. The design and fabrication of surface coatings with anti-friction properties represent a promising way for the reduction of energy dissipation and detrimental environmental effects on power losses caused by fluid friction. Following a biomimetic approach, we designed hybrid organic-inorganic layers able to generate hierarchically organized coatings with advanced repellence against water and oils. In order to assess the anti-friction properties of the amphiphobic (both superhydrophobic and oleophobic) surfaces, the influence of surface topography on the lubrication performance of an axial piston pump has been investigated with a complete multi-scale description of the frictional dissipation and an ad-hoc developed test ring simulating operative conditions. Compared to the uncoated slippers we observed a significant reduction in friction coefficient (up to 27%) which remains constant even after endurance test of 20 hours.

### **3481790: In Vitro Wear Test of Pyrolytic Carbon Against Cartilage for Shoulder Hemiarthroplasty**

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Interposition prostheses made of pyrolytic carbon (PyC) are implanted in the shoulder as hemiarthroplasty, i.e. they articulate against cartilage as counterbody<sup>1,2</sup>. Reportedly, PyC has good biocompatibility (anti-thrombogenic properties, non toxicity and allergic responses), and excellent fatigue and wear resistance<sup>3-5</sup>. The aim of this project, a collaboration between RUSH and LaMCos, is the comparison of tribological properties of PyC versus traditional biomaterials (alumina ceramic and cobalt-base alloy). All these materials were articulated against living cartilage explants in biomimetic synovial liquid containing phospholipid vesicles filled with hyaluronic acid<sup>6</sup>. Cartilage degradation was evaluated by sulfated glycosaminoglycans and hydroxyproline dosage. The surface of the counterbody was investigated as well by dosage of adsorbed oxidized phospholipids. A new viability test, based on the mitochondrial activity of chondrocytes in tissues was introduced as well. Initial results suggest that CoCrMo induces the greatest cytotoxicity, and that otherwise no difference were observed. Further tests are required to solidify the trend.

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