Tribology and Mechanics of Coatings and Surfaces
Room Palm 3-4 - Session MC1-1-ThA

Friction, Wear, Lubrication Effects, & Modeling I

Moderators: Pierluigi Bilotto, TU Wien, Austria, Michael Chandross, Sandia National Laboratories, USA

1:20pm **MC1-1-ThA-1 Solid Lubrication in Thin Films: Mechanisms, Materials, and Performance***, Daniel Pölzlberger,* Institute of Materials Science and Technology, TU Wien, Austria*; Rainer Hahn, Tomasz Wojcik, Philip Kutrowatz,* Christian Doppler Laboratory for Surface Engineering of High-performance Components, TU Wien, Austria*; Klaus Böbel, Julien Keraudy,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials GmbH, Germany*; Philipp G. Grützmacher, Carsten Gachot,* Institute of Design Engineering and Product Development, Research Unit Tribology, TU Wien, Austria*; **Helmut Riedl**,* TU Wien, Institute of Materials Science and Technology, Austria **INVITED**

Tribological contacts play an essential role in the prevalent and required endeavor for increased sustainability and efficient use of resources. Considering the energy losses related to friction and wear, a huge possibility of saving resources, energy, and CO_2 is often overlooked. Here, solid lubricants are an attractive option, especially for applications pushing their conventional liquid counterparts to their thermal and chemical stability limits – typically at elevated temperatures above 200 °C or under extreme conditions excluding liquids (i.e. space industry, semiconductors, or life science). Therefore, this study examines different solid lubrication concepts in thin film materials, classifying them concerning predominant mechanisms, application ranges, and performance.

As a starting point, carbon-containing thin film materials will be discussed comprising diamond-like carbon (DLC) coatings and non-reactively sputter deposited transition metal (TM) carbide thin films (i.e., HfC, TaC, or WC). Here, advances in PVD growth techniques (i.e., HiPIMS) and their impact on tribological performance are in focus. Furthermore, insights on the limits of carbon as the source for solid lubrication will be given by a set of high-resolution characterization techniques (i.e., HR-TEM, APT, etc.). The second part presents an alternative class of TM dichalcogenide coating materials (compared to MoS_2) and their in-situ formation. In detail, in an innovative approach, selenium nanopowders are converted in-situ into lubricious 2D selenides on sliding W and Mo films, achieving a coefficient of friction (COF) down to 0.1 in ambient air. This in-situ formation is an exciting concept, especially for extreme environmental conditions. Nevertheless, further advances in solid lubricants are required to overcome the limitations for high-temperature applications (above 450 °C). Here, a concept on B_2O_3 formation in TM borides (i.e., $TiB_{2\pm z}$ or $WB_{2\pm z}$) leads to a drastic reduction of COF from 0.6 to 0.2 at 500 °C (and higher temperatures), highlighting the capabilities of boron-containing thin films in high-temperature tribological contacts.

In summary, the different concepts of solid lubrication in thin film materials emphasize the potential of exploring new materials and the need for an in-depth understanding to push these materials in potential applications.

2:00pm **MC1-1-ThA-3 Study of Transparent Coatings for the Preservation of Colored Titanium Surfaces***, Sarah Marion, Renée Charrière,* Mines Saint-Etienne, France*; Clotilde Minfray,* Ecole Centrale de Lyon - LTDS, France*; Laurent Dubost,* HEF - IREIS, France*; Jenny Faucheu,* Mines Saint-Etienne, France*; **Vincent Fridrici**,* Ecole Centrale de Lyon - LTDS, France

Although titanium is not a noble metal, it is increasingly attracting interest from the luxury industry (jewelry, watches, packaging) due to its lightweight, hypoallergenic properties, and especially the wide range of colors it can display when coated with a thin layer of TiO_2. However, its application in luxury products remains limited because these colors tend to lack durability. Improving the wear resistance of these colored TiO_2 layers, and in particular preserving the original color, is a critical challenge for luxury jewelry.

The interference-based nature of titanium's color makes it highly sensitive to changes in oxide layer thickness, as well as to variations in the oxide layer's chemical composition and internal structure, which can alter its refractive index. Tribological tests conducted on thin titanium oxide layers, using a100Cr6 steel ball in both dry conditions and with artificial sweat, demonstrated a clear correlation between color changes due to friction and a reduction in oxide layer thickness in both environments.

An experimental study of the wear resistance of several potential protective coatings deposited on oxidized titanium samples is carried out in order to preserve the color of the samples. Three coatings—SiAlON, Si_3N_4, and a commercial hydrophobic coating—were examined for their wear resistance in both dry and artificial sweat conditions, as well as for their transparency and surface wettability. The challenge is to have a coating that is not only transparent but also resistant to wear in both dry and sweat-exposed conditions and insensitive to fingerprints.

Thus, the color variation before and after coating, the surface wettability of the coating with water and sebum, as well as its resistance to dry friction and friction in the presence of artificial sweat against a 100Cr6 steel ball, will be analyzed and compared to those of uncoated TiO_2 to assess the performance of the coatings.

2:20pm **MC1-1-ThA-4 Beyond Graphene: A ML-Assisted High-Throughput Molecular Dynamics Framework for Screening 2D Materials for Tribological Applications***, **Matteo Valderrama**, Daniele Dini, James Ewen,* Imperial College London, UK*; Nicolas Fillot,* INSA de Lyon, France

2D materials, with their unique atomic structures and tunable properties, have shown immense potential for achieving superlubricity (COF < 0.01) in sliding contacts. However, the vast design space of these materials presents a significant challenge in identifying optimal candidates for specific tribological applications. To date, only around ten 2D materials have been extensively studied for their tribological properties. This work explores a framework for applying machine learning (ML) assisted high-throughput molecular dynamics (MD) simulations to accelerate the discovery of high-performance 2D materials for tribological applications. 2D materials exhibit fundamentally different frictional behavior compared to their bulk counterparts, a phenomenon that can be observed at the atomic scale. To study this, our framework will computationally screen the tribological performance of thousands of 2D materials. By streamlining simulation cell generation and optimization, this framework facilitates the processing of tens of thousands of MD simulations. Combined with the recent advancements in GPU-powered simulations, this project could transform high-throughput MD, especially through the hybridization of both the computational approaches (CPU vs. GPU) and the implementation of interatomic potentials. The extracted tribological data will be used to train ML models, such as regressive random forests, LSTMS, and LLMs, to predict the performance of new materials. Our goal is to establish correlations between specific material properties and atomic friction mechanisms, gaining deeper insights into the underlying causes of atomic friction. We anticipate that this project will revolutionize the field of 2D materials by accelerating the design, prototyping, and experimental validation of materials that demonstrate robust superlubricity, making research more accessible and reproducible, and ultimately paving the way for their widespread adoption in various applications. In this presentation, I will delve into the details of our framework, demonstrate its validity, and present preliminary results on predicting friction in 2D materials based on their intrinsic properties.

2:40pm **MC1-1-ThA-5 Modelling Complexities of Tribocorrosion Processes: Evaluation and Validation***, **Avirup Sinha**,* University of Illinois at Chicago, USA*; Feyzi Hashemi,* Flinders University, Australia*; Maansi Thapa, Bill Keaty, Yani Sun,* University of Illinois at Chicago, USA*; Reza Hashemi,* Flinders University, Australia*; Mathew T. Mathew,* University of Illinois at Chicago, USA

Introduction:

Biomedical implants are vital medical devices surgically placed to replace or support damaged tissues and organs. Modular implants, such as hip replacements, improve adaptability for diverse patients but introduce challenges like tribocorrosion—a complex interaction of tribology and corrosion. Tribocorrosion releases debris, ions, and particles into surrounding tissues, causing reactions, systemic toxicity, and infections. Biocompatible materials like Ti6Al4V are commonly used in implants. Although various experimental methods exist to study tribocorrosion, limited mathematical modeling efforts have been undertaken. This study reviews available models to identify those most suitable for implant applications, with two aims: a) validating model efficiency using literature data, and b) conducting experiments to generate data for further validation.

Methodology:

Aim 1: Electrochemical current evolution is a key measure of tribocorrosion. Models like "Olsson and Stemp," "Feyzi and Hashemi," and the Uhlig model predict tribocorrosion currents, but their efficiency remains insufficiently tested. Data from M.T. Mathew et al.'s "Tribocorrosion Behaviour of

TiCxOy" was selected for its robust dataset, clear graphical representation, and systematic evaluation across varying voltages, ensuring analytical versatility. Aim 2: Fretting-corrosion experiments were conducted using a custom-built tribocorrosion apparatus (Pin- on-flat) to validate models against experimental outcomes. Materials included Ti6Al4V and CoCr bases with a Zr pin. Testing was performed in 0.9% saline at 83N load and ±6mm amplitude at 1Hz frequency.

Results:

Aim 1 demonstrated that Mischler's model outperformed Olsson and Stemp's in predicting experimental data. While Olsson's model worked well at -0.5V, it struggled at +0.5V due to assumptions about voltage- dependent oxide film growth, making it better suited for lower voltage predictions. Aim 2 revealed Feyzi and Hashemi's model best predicted tribocorrosion behavior, though significant variance highlighted the need for refined assumptions. Olsson and Stemp's model showed promise with adjustments to variables like oxide layer thickness, emphasizing its role in tribocorrosion modeling.

Conclusions:

The study concludes that tribocorrosion current is influenced by multiple factors, and model predictions improve with accurate variable inputs. Further research is needed to refine models, including developing experimental procedures to determine assumed variable values (e.g., asperity radius) and creating real- time computational models to compare experimental and predicted results.

3:00pm **MC1-1-ThA-6 Electrification of Ti:MoS_2 Coatings for Tribological Applications***, **Newton K. Fukumasu**,* Institute for Technological Research of Sao Paulo State, Brazil*; Miguel R. Danelon, André P. Tschiptschin, Izabel F. Machado, Roberto M. Souza,* University of São Paulo, Brazil

Next-generation adaptive coatings for heavy-loaded mechanical transmission systems enhance durability and efficiency by coupling external parameters, such as electrical conditions, with tribological performance, particularly relevant for electric vehicle powertrains and energy generation systems, where controlling friction and wear is crucial for improving operational efficiency. Also, in those systems, stray currents could be used for improving tribological aspects of mechanical systems. Coatings of transition metal dichalcogenides, such as molybdenum disulfide, promote excellent solid lubrication under high contact stresses and pure sliding conditions, but higher wear rates compromise coating durability. Metal-doping MoS_2 coatings allows the optimization of mechanical properties, including hardness and elastic modulus, promoting an amorphous coating structure and engineered coating bandgap. In this work, Ti:MoS_2 coatings were deposited using a pulsed D.C. magnetron sputtering, with doping levels controlled by varying the power applied to Ti target. Tribological tests under electrified reciprocating conditions were conducted with uncoated AISI 52100 balls against Ti:MoS_2 coated glass plates. Ti concentration was varied between 10 at% and 20 at% and electrified tests conditions considered positive, negative, and non-electrified contact with, when applied, a constant electric current of 100 mA. Ball movement frequency was set at 0.375 Hz with 4 mm stroke. Results indicated that friction was reduced under electrified conditions, particularly for coatings with lower Ti concentrations. Raman spectroscopy revealed recrystallized MoS_2 inside wear tracks, suggesting tribo-induced structural adaptation. Wider wear tracks and greater surface damage were observed when ball was positively charged. Results suggest that the electric field may promote differential migration of Mo, S, and Ti species, altering the tribofilm composition and morphology formed at the ball surface. This selective adsorption on the ball further enhances the formation of MoS_2-rich regions, in which tribochemical reactions, enhanced by the electric current, may favor MoS_2 retention and regeneration at lower Ti concentrations, while higher Ti concentrations disrupt the lubricating behavior. The integration of tribology and electrification may lead to enhanced efficiency and durability of critical mechanical systems with selective surface chemistry and adaptive tribological performance.

3:20pm **MC1-1-ThA-7 Nanoscale Wear of Metallic Multilayers - the Effect of Interface***, **Tomas Polcar**, Ahmed AlMotasem,* Czech Technical University in Prague, Czech Republic

Extensive large molecular dynamics simulations (MD) were conducted to investigate the impact of different Zr/Nb interface orientations on the friction/wear behavior of Zr/Nb multilayers. The primary cause of plastic deformation of the Nb layer was dislocations and BCC twinning, while Zr layers deformed via dislocations and intrinsic stacking faults. The Zr/Nb exhibited better tribological properties, such as lower COF, higher scratch hardness, and improved wear resistance compared to their single-crystal counterparts. The interface structure was analyzed, and its blocking strength was discussed. tailoring them to achieve desired properties for specific applications.

The simulations of friction and wear were compared with experimentally obtained nanoscratches on Zr/Nb multilayers with a periodicity of 6 nm prepared by magnetron sputtering. The wear was evaluated by AFM, structure by STEM and XRD. Qualitative agreement with experiments demonstrates predictive power of MD simulations in tribology.

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