Tribology and Mechanics of Coatings and Surfaces
Room Palm 3-4 - Session MC1-2-FrM

Friction, Wear, Lubrication Effects, & Modeling II

Moderators: Julien Keraudy, Oerlikon Balzers Coating AG, Liechtenstein, **Pantcho Stoyanov**, Concordia University, Canada

8:00am **MC1-2-FrM-1 Linking Atomic-Scale Surface Structure and Friction via Multiscale Modelling: The Case of Carbon-Based Coatings and Tribofilms***, **Gianpietro Moras [gianpietro.moras@iwm.fraunhofer.de]**,* Fraunhofer IWM, MicroTribology Center TC, Germany **INVITED**

Carbon surfaces play a fundamental role in tribology. There is not only the case of carbon-based coatings, but also the less obvious case of low-friction, carbon-based tribofilms deposited on other materials by liquid or solid lubricants. In all cases, friction in dry and boundary lubrication conditions depends on the atomic structure of the sliding surfaces. A stable chemical passivation of surface dangling bonds is a prerequisite for low friction and wear. However, even subtle changes in surface chemistry can cause the friction coefficient of passivated carbon interfaces to vary significantly. In this talk, I will present the results of multiscale simulation studies that combine quantum mechanics, molecular dynamics and contact mechanics to shed light on the relationships between the chemical structure of carbon surfaces and friction.

I will initially focus on superlubricity (friction coefficient < 0.01) with diamond-like carbon coatings and silicon nitride. Stable superlubricity over a wide range of operation conditions has been recently achieved at Fraunhofer IWM in plain-bearing test rigs using glycerol as a lubricant. Hydrodynamic superlubricity with glycerol is possible at high temperature and facilitated by the presence of water. However, the mechanisms responsible for superlubricity in boundary lubrication with glycerol are still under debate. Our simulations reveal a complex mechanochemical process involving the tribochemical decomposition of glycerol molecules at surface asperity contacts, the plastic deformation of the resulting H-, O- or N-containing amorphous carbon tribofilm and the formation of partially aromatic surface regions. These smooth and unreactive surfaces enable superlubricity even when asperity contacts run dry or are separated by nanometric, highly viscous glycerol films.

In the second part of my talk, I will extend the study to the effects of boron and fluorine. Our simulations suggest that hydroxyl groups that normally passivate carbon surfaces in humid environments can be activated by boron and form B−O dative bonds across the tribological interfaces, leading to a mild friction increase. Surface passivation by C−F bonds, instead, is very stable. This is the basis of the exceptional tribological properties of some perfluorinated carbon materials, but also of their accumulation in the environment and in biological systems. Our simulations provide answers to open questions about their friction mechanisms that may be useful in the search for alternatives: Why are perfluorinated carbon surfaces polar and hydrophobic? Why are they more slippery than their hydrogenated analogues? Why is PTFE non-sticky but forms transfer films on PTFE-lubricated steel surfaces?

8:40am **MC1-2-FrM-3 Impact of Gaseous Environments on the Tribological Performance of Steel and Advantages of DLC Coatings***, **Pierre-Francois Cardey [Pierre-Francois.Cardey@cetim.fr]**,* Cetim, France **INVITED**

The tribological performance of materials is strongly influenced by the gaseous environment, where composition and pressure alter wear and friction mechanisms. In particular, the energy and transportation industries are paying increasing attention to hydrogen-related issues due to its potentially embrittling effects and impacts on tribological performance. At CETIM, a pin-on-disc tribometer was developed to analyze these interactions under various gaseous atmospheres across a wide range of temperatures and pressures.

This study focuses on two steel grades (high carbon and chromium steel 52100, and austenitic stainless steel 316L), tested in nitrogen, helium, and hydrogen atmospheres, with variations in contact pressure, temperature, and sliding speed. The results highlight how these environments affect the formation of protective oxide layers, which play a key role on friction and wear. The effects of hydrogen are also specifically studied due to its embrittling and reducing properties.

In this context, Diamond-Like Carbon (DLC) coatings emerge as a promising solution, acting both as a barrier to hydrogen diffusion and as a tribological enhancement in harsh gaseous environments. This study provides a comprehensive approach to optimizing material selection and surface treatments to improve the durability of components exposed to challenging industrial gaseous atmospheres.

9:20am **MC1-2-FrM-5 Study of Microabrasive Wear on TiB2/TiB Hard Layer Formed on Ti6Al4V Alloy.***, **Marco A Melo-Pérez [mmelop@ipn.mx]**,* Av. Instituto politécnico nacional, Mexico*; German A. Rodríguez-Castro, Alfonso Meneses-Amador, Ezequiel A. Gallardo-Hernández, Israel Arzate-Vázquez, José A Nieto-Sosa,* Instituto Politécnico Nacional, Mexico

Micro-abrasion wear resistance of TiB2/TiB layers was studied by ball cratering tests formed on Ti_6Al_4V by powder-pack boriding. The boriding process was carried out at 1273 K over 5 and 20 h of treatment resulting in the formation of TiB2/TiB layer with a maximum thickness of 10 µm. The layers' mechanical characterization was carried out using Berkovich instrumented indentation, obtaining hardness greater than 2.5 GPa.The wear coefficient of TiB_2 phase was evaluated by micro-abrasion tests using SiC particles dissolved in deionized water as abrasive slurry. The results demonstrated that the titanium borides have wear coefficients higher than Ti_6Al_4V and improve their micro-abrasion wear resistance. Furthermore, a wear-mode map was developed to identify the two and three body abrasion mechanisms and the transition between them modifying the concentration of SiC in the slurry and the magnitude of applied load.

9:40am **MC1-2-FrM-6 Tribology of Protective CrN Coatings in Arctic Environmental Conditions***, **Forest Thompson [forest.thompson@sdsmt.edu]**, Elyse Jensen, Nathan Madden, Grant Crawford,* South Dakota School of Mines and Technology, USA

The friction and wear behavior of protective CrN coatings has been shown to be highly sensitive to Arctic environmental conditions, such as the combination of cold temperatures (<20 °C) with low dew points (<-30 °C). To advance the mechanistic understanding of the tribological response of CrN to Arctic environments, the relationships between coating architecture, environmental conditions, coefficient of friction, and wear resistance were investigated. A series of CrN coatings were deposited onto stainless steel substrates with varying adhesion layer compositions (Cr, Ti, CrN) by reactive pulsed DC magnetron sputtering. Microstructural characterization of the as-deposited coatings was conducted via laser scanning confocal microscopy, electron microscopy, energy dispersive x-ray spectroscopy, and x-ray diffraction. Linearly reciprocating sliding wear tests were conducted using a ball-on-flat tribometer. The tribometer was equipped with an active cooling stage and a dry air source to achieve coating surface temperatures and environmental dew points representative of conditions that would be encountered in Arctic service environments. After tribological testing, focused ion beam milling and transmission electron microscopy were utilized to analyze specific sites within wear scars and to characterize wear debris structure. The results from this work contribute to efforts related to the design of protective coatings for extreme environments, such as those encountered at Earth's polar regions.

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