


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 , 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 Effects of Graphene Additives on the Mechanical Properties and Corrosion Resistance of Plasma Electrolytic Oxidation Coatings on AZ31B Magnesium Alloy**, **Guan Zhong Chen** [M11188020@o365.mcut.edu.tw], Department of Materials Engineering, Ming Chi University of Technology, Taiwan., Taiwan; **Chuan Ming Tseng**, Center for Plasma and Thin Film Technologies, Ming Chi University of Technology, Taiwan., Taiwan

Graphene, as a two-dimensional layered material, exhibits excellent electrical conductivity and superior friction and wear resistance, making it widely applicable in various industries. In this study, the ceramic composite coatings on AZ31B magnesium alloy were prepared by using plasma electrolytic oxidation (PEO) in alkaline solutions with sodium phosphate, sodium silicate, potassium fluotitanate and graphene additions. The effect of graphene content on mechanical properties and corrosion resistance of PEO coatings on AZ31B magnesium alloy was investigated. The microstructural characteristics and compositional analysis of the PEO coatings were examined by using field emission scanning electron microscopy (FE-SEM), X-ray energy dispersive spectroscopy (EDS), and X-ray diffraction (XRD). The micro-Vickers hardness tester, nanoindentation instrument and a pin-on-disk tribometer were employed to measure the hardness and wear resistance of PEO coatings. The potentiodynamic polarization measurements and salt spray test were conducted to evaluate the corrosion behaviors of PEO coatings in NaCl containing circumstances. The experimental results revealed that as increasing the graphene content

from 25 mg/L to 75 mg/L, the thickness of PEO coating increased from 24.7 μm to 37.5 μm and the porosity decreased from 13.03% to 7.82%. The results of XRD and SEM-EDS indicated that the PEO composite coatings were mainly composed of MgO and Mg₂SiO₄. The hardness of PEO coating was increased with increasing the graphene content and the optimal hardness 1696 HV attained on the PEO coating with 75 mg/L of graphene addition. The potentiodynamic polarization curves in a 3.5 wt% NaCl solution showed the corrosion current density decreased with increasing graphene addition and the highest polarization impedance achieved for the PEO coating with 75 mg/L of graphene addition. Furthermore, the results of salt spray test after 14 days-exposure indicated that the PEO coatings with graphene addition exhibited fewer and smaller corrosion pits as compared to the PEO coating without graphene addition. In summary, the mechanical properties and corrosion resistance of PEO coatings were pronouncedly improved by graphene nanosheets incorporation.

9:00am **MC1-2-FrM-4 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 ($< 20\text{ }^\circ\text{C}$) with low dew points ($< -30\text{ }^\circ\text{C}$). 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.

9:20am **MC1-2-FrM-5 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.

10:00am **MC1-2-FrM-7 Sliding Wear Behavior of Borided Ti₆Al₄V Alloy Under Dry Conditions and Simulated Body Fluids**, **J. A. Nieto-Sosa** [antonio.nieto1094@gmail.com], **G. A. Rodríguez-Castro**, **A. Meneses-Amador**, INSTITUTO POLITECNICO NACIONAL, Mexico; **E. E. Vera-Cárdenas**, INSTITUTO TECNOLÓGICO DE PACHUCA, Mexico; **R. Pérez-Pastén-Borja**, **N. A. Hernández-Rosas**, INSTITUTO POLITECNICO NACIONAL, Mexico

This study investigated the resistance to wear of borided Ti₆Al₄V alloy under dry conditions and in calf serum as simulated body fluid. The layers

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formation was conducted by powder-pack boriding at 1100 °C for 5 and 20 h of exposure time. The layer thicknesses less than 11 μm and hardness around 25 GPa were determined by optical microscopy and instrumented indentation, respectively. Through X-ray diffraction, TiB₂ and TiB phases are identified, and the distribution of the chemical elements of B, Ti, Al and V are analyzed by energy-dispersive spectroscopy (EDS). Reciprocating sliding tests were performed with an ball of 6.35 mm of diameter as counterpart, setting a sliding distance of 100 m and loads of 10 and 20 N for both conditions. The tribological results show that the wear rate decreases in the hardened titanium. In addition, the effects of the SBF are studied on the friction coefficient and wear mechanisms.

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