

## Tribology and Mechanics of Coatings and Surfaces

### Room Palm 3-4 - Session MC1-2-FrM

#### Friction, Wear, Lubrication Effects, & Modeling II

Moderator: Klaus Boebel, Oerlikon Surface Solution AG, Liechtenstein

8:20am **MC1-2-FrM-2 Active Friction and Wear Control in a-C:Cr Films: Electrical Current and Polarity Effects on Catalytic Graphitization**, **Newton K. Fukumasu** [[newton.fukumasu@usp.br](mailto:newton.fukumasu@usp.br)], **Miguel R. Danelon**, University of São Paulo, Brazil; **Abrar Faiyad**, **Ashlie Martini**, University of California Merced, USA; **Cherlio Scandian**, Federal University of Espirito Santo, Brazil; **Roberto M. Souza**, University of São Paulo, Brazil

Diamond-Like Carbon (DLC) films are established protective coatings for severe contact conditions, yet their tribological response under active electrical currents involves under-explored physical mechanisms. This study investigates the friction and wear behavior of Cr-doped (a-C:Cr) and undoped a-C films under reciprocating sliding with simultaneous electrical current passage. Tests were performed in dry conditions, using AISI 52100 steel balls against coated glass substrates under anodic (positive plane) and cathodic (negative plane) polarizations, applying a 10 N normal load, 4 mm stroke, and a constant current of 100 mA for the electrified cases. While undoped DLC exhibited inert behavior, resulting in a friction coefficient (COF) of 0.15 regardless of electrical conditions, Cr-doped films demonstrated a friction reduction, down to 0.05, and significant responsiveness to the applied current. Although instrumented indentation and microscopy indicated slightly lower hardness and more visible wear marks for a-C:Cr compared to the undoped film, the tribological behavior is attributed to a local shear-induced phase transformation mechanism. Raman spectroscopy of the a-C:Cr wear tracks under cathodic polarization revealed an intense 2D peak, characteristic of ordered, multilayer graphene-like structures. This result provides evidence that Cr catalytically lowers the activation energy for graphitization, activated by local heating and electron flow. Conversely, anodic polarization resulted in clean wear tracks and stable low friction, suggesting a distinct equilibrium between tribofilm formation and oxidative removal. Reactive Molecular Dynamics simulations supported these findings, elucidating atomistic pathways where Cr clusters facilitate bond rehybridization under combined shear and electrochemical stress. These results demonstrate that the tribological performance of a-C:Cr can be actively tuned, enabling "on-demand" low-friction regimes through electrically assisted catalytic graphitization.

8:40am **MC1-2-FrM-3 Tribological Performance of Sputter-Deposited MoS<sub>2</sub> Coatings with Varying Process Gases**, **Tomas Babuska** [[fbabus@sandia.gov](mailto:fbabus@sandia.gov)], **Alexander Mings**, **Steven Larson**, **John Curry**, **David Adams**, Sandia National Laboratories, USA

Sputter-deposited molybdenum disulfide (MoS<sub>2</sub>) coatings have been used for decades in aerospace applications due to their ultra-low steady-state coefficients of friction ( $\mu_{ss} < 0.05$ ). Developing MoS<sub>2</sub> coatings for demanding applications with predictable and reliable performance over time (i.e., high-quality) requires tuning the coating microstructure through process variations. In this work, we explore process-structure-property-performance relationships of pure MoS<sub>2</sub> solid lubricant coatings where coatings are sputter deposited using different process gases. Helium, krypton, neon, argon and xenon are used to sputter deposit MoS<sub>2</sub> of varying morphologies, and the impact on critical performance traits such as initial friction, run-in, and aging resistance are studied. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

9:00am **MC1-2-FrM-4 Effect of Ta Content in ta-C:Ta Coatings on the Machining Performance of Aluminum Alloy**, **Kosuke Suzuki** [[kousukes@mmc.co.jp](mailto:kousukes@mmc.co.jp)], Mitsubishi Materials Corporation, Japan; **Takayuki Tokoroyama**, **Ruixi Zhang**, **Noritsugu Umehara**, Nagoya University, Japan; **Shun Sato**, **Kenji Yumoto**, Mitsubishi Materials Corporation, Japan **INVITED**

In recent years, demand for lightweight materials in the automotive and aerospace industries has increased, leading to a growing need for machining aluminum alloys. In aluminum alloy machining, Diamond-Like Carbon (DLC) coatings—especially hydrogen-free tetrahedral amorphous carbon (ta-C) coatings—are widely used due to their excellent wear resistance and low friction, which help suppress material adhesion and tool wear caused by hard Si particles in the alloy.

However, under more severe machining conditions, further improvements in coating performance are required to extend tool life, especially in terms of wear resistance and delamination resistance. One of the representative approaches for such performance enhancement is the addition of transition

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metal elements to DLC coatings, and numerous studies have been reported in this area. Among these, tantalum (Ta) is known to form strong covalent bonds with carbon and is expected to achieve both mechanical strength and improved adhesion strength through the reduction of residual compressive stress. Nevertheless, studies on its influence on machining performance remain limited.

In this study, tantalum-doped ta-C (ta-C:Ta) coatings with varying Ta contents were fabricated, and the correlation between Ta content and coating properties, as well as its effect on the drilling performance of aluminum alloy (ADC12), was systematically evaluated.

For each coating, microstructural analysis and residual stress measurements were conducted, along with ball-on-disk friction tests and scratch tests. Additionally, aluminum alloy cutting tests were performed to evaluate wear resistance and cutting force. As a result, the friction coefficient and specific wear rate tended to increase with higher Ta content in the friction tests. On the other hand, the scratch tests showed an increase in critical load, and a correlation between critical load and residual compressive stress was confirmed. Observations of the scratch marks revealed that ta-C:Ta coatings exhibited smaller delamination areas compared to undoped ta-C coatings. The dispersed structure of TaC nanocrystals observed in the ta-C:Ta coatings is suggested to reduce delamination propagation and contribute to improved toughness.

In the cutting tests, the coating containing 1.1 at.% Ta demonstrated the best wear resistance and lowest cutting force by significantly suppressing chipping while maintaining resistance to abrasive wear. These results suggest that controlling residual stress through appropriate Ta addition and enhancing toughness via fine TaC structures are effective strategies for improving tool life in aluminum alloy machining.

10:20am **MC1-2-FrM-8 Effects of Silver Nitrate Additives on the Antibacterial and Corrosion Behaviors of Plasma Electrolytic Oxidized AZ31 Magnesium Alloy**, **Bo-Xuan Zheng** [[rick910823@gmail.com](mailto:rick910823@gmail.com)], **Chuan-Ming Tseng**, Ming Chi University of Technology, Taiwan, Republic of China

AZ31 magnesium alloy exhibits excellent biodegradability and biocompatibility, making it a promising candidate for temporary biomedical implants. Nevertheless, its rapid degradation and insufficient corrosion resistance severely limit its direct clinical application. In this study, the bioceramic composite coatings on AZ31 magnesium alloy were prepared by using plasma electrolytic oxidation (PEO) under bipolar power mode in alkaline solutions with sodium phosphate, sodium silicate, potassium fluotitanate and silver nitrate (AgNO<sub>3</sub>) additions. The effect of AgNO<sub>3</sub> content on antibacterial and corrosion behaviors of PEO coatings on AZ31 magnesium alloy was investigated. The microstructural characterizations of the AgNO<sub>3</sub>-incorporated PEO coatings were identified by XRD, SEM-EDS and EPMA. The adhesion and wear resistance of PEO coatings were evaluated using scratch testing and pin-on-disk wear tests, respectively. The potentiodynamic polarization measurements were conducted to evaluate the corrosion behaviors of PEO coatings in simulated body fluid (SBF) solutions. The antimicrobial properties of PEO coatings were carried out by measuring the numbers of *Escherichia coli* bacterial colony after various incubation durations. The XRD patterns reveal that the PEO coatings are mainly composed of MgO (inner layer) and Mg<sub>2</sub>SiO<sub>4</sub> (outer layer). Cross-sectional SEM-EDS mapping images confirm that Ag elements are well dispersed near surface of PEO coatings. The highest adhesion strength (~36 N) and the lowest wear rate ( $5.5 \times 10^{-6} \text{ mm}^3/\text{N m}$ ) can be achieved for the PEO coating with 0.2 g/L AgNO<sub>3</sub> incorporated. However, the potentiodynamic polarization curves display that the PEO coatings, as compared to AZ31 magnesium alloy, exhibit higher corrosion resistances in SBF solutions. Furthermore, the PEO coating with 0.2 g/L AgNO<sub>3</sub> addition shows the optimal corrosion resistance due to its lowest corrosion current density ( $1.07 \times 10^{-8} \text{ A/cm}^2$ ). Furthermore, the antibacterial efficiency of the PEO coatings is significantly improved with increasing AgNO<sub>3</sub> additives. More interestingly, all the PEO coatings with various AgNO<sub>3</sub> incorporated exhibit a 100% antibacterial efficiency to *Escherichia coli* after incubation in 45 minutes. In summary, the adhesion, wear resistance, antibacterial efficiency and corrosion resistance of PEO coatings on AZ31 magnesium alloy can be pronouncedly improved by AgNO<sub>3</sub> additions, highlighting their potential for biodegradable implant applications.

Keywords: PEO, AZ31, Silver nitrate, Corrosion resistance, SBF.

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10:40am MC1-2-FrM-9 Experimental Investigation of Friction, Wear, and Dielectric Behavior of Hybrid Polymer Nanocomposites for Insulated Bearings with Machine Learning Assisted Optimization, *Unnati Joshi [unnatajoshi@gmail.com], Anand Joshi, Vishal Mehta, Jaivik Pathak, Pranav Rathi*, Parul University, India

The present research reports the development and comprehensive investigation of polymer based hybrid nanocomposites composed of Graphene Oxide (GO) and Copper Oxide (CuO) nanoparticles reinforced Polyether ether ketone (PEEK), designed for multifunctional efficacy in advanced high speed electromechanical system applications, including insulated bearings. The objective was to improve the friction-wear characteristics and dielectric properties of the base PEEK polymer. The suitability of the hybrid nanocomposites for insulated bearing applications were evaluated by examining the dielectric constant, dielectric loss, wear rate, and coefficient of friction. Structural and morphological properties were characterized using SEM, EDS, XRD, and FTIR. In this study, the friction, wear and dielectric properties of PEEK based nanocomposites containing 5 wt% Graphene Oxide and varying Copper Oxide nanoparticle contents (1 to 5 wt%) were experimentally investigated. Among all the compositions that were examined, the nanocomposite containing 5 wt.% GO and 5 wt.% CuO nanoparticles demonstrated the highest  $R^2$  value of 88% for wear resistance and 93% for coefficient of friction, thereby validating its optimal performance level and operational stability. The simultaneous enhancements that result from the combination of CuO and GO are indicative of improved surface strength. Furthermore, the machine learning regression models, including Random Forest, XGBoost, and Extra Tree, have exhibited exceptional predictive capabilities for wear and friction forces. The Extra Tree model, in particular, achieved near-perfect accuracy ( $R^2 = 0.9999$ ) and identified load as the most influential factor. Also, the dielectric constant ( $\epsilon'$ ) and dielectric loss ( $\epsilon''$ ) were predicted and modelled using these machine learning models. The analysis demonstrated that the highest  $\epsilon'$  was achieved at 2 wt% Copper Oxide as a result of increased interfacial polarisation, while the most stable dielectric loss ( $\epsilon''$ ) was achieved at 3 and 4 wt% Copper Oxide. The Extra Trees algorithm consistently exhibited superior predictive accuracy and generalisation capability among all the models. This demonstrates that the wear resistance, coefficient of friction, and dielectric behaviour of the composites, were substantially influenced by the synergistic interaction between Graphene Oxide and Copper Oxide nanoparticles. This research advances durable, high performance insulating materials for next-generation electromechanical systems, supporting SDG 9. It also promotes SDG 12 by supporting the design of affordable, durable materials that reduce material waste and enhance industrial component energy efficiency.

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