Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room San Diego - Session E1-3-FrM
Friction, Wear, Lubrication Effects, and Modeling IV

Moderators: Nazlim Bagcivan, Schaeffler Technologies GmbH & Co. KG, Germany, **Carsten Gachot**, Vienna University of Technology, **Tomas Polcar**, Czech Technical University in Prague, Czech Republic

8:00am **E1-3-FrM-1 Numerical and Experimental Analyses on the Influence of Irregular Columnar Boundaries on Mechanical and Tribological Behavior of a WC/C Coating**, ***Cassiano Bernardes***, *N Fukumasu, R Souza, I Machado,* University of São Paulo, Brazil

Many commercial coating deposition systems produce microstructures with defects that can affect the tribological performance of a given component. Instabilities during the deposition process or variations on local surface topography can lead to macroscale defects, such as irregular columnar boundaries. Those columnar defects can present interfacial discrepancies between two consecutive columns, leading to local lower mechanical and fracture properties. This work explores the influence of irregular columnar growth of a Tungsten Carbide / Carbon (WC/C) multilayer coating, on local and global tribological behavior. The samples consisted of a commercial version of a WC/C coating deposited onto polished AISI H13 discs and AISI 52100 balls. Mechanical, fracture and microscale tribological behaviors were analysed using a Bruker TI950 triboindenter. Macroscale tribological behavior was evaluated by reciprocating tests using the Optimol SRV v4 tribometer in the ball-on-disk configuration. X-ray diffraction (XRD), x-ray photoemission spectroscopy (XPS) and Raman spectroscopy techniques were used to characterize the coating microstructure. Numerical simulations of the microscale scratch test, using the digital tribology package TRIBOCode, allowed the analyses of the local columnar irregularities on the tribological behavior of the coating. The macroscale reciprocating results showed variable tribological behavior of the coating induced by the defects, in which only part of the tests presented coating failure (cohesive cracks and spallation). XRD and XPS analyses indicated a presence of crystalline phases of type WC_{1-x}, while the presence of amorphous carbon matrix was identified during the Raman analyses. The numerical simulations indicated a correlation between the orientation of the mechanical and fracture properties of the irregular columnar structures and boundaries and the scratch direction, which could lead to selective failure modes of the coating.

8:20am **E1-3-FrM-2 Structure, Mechanical and Tribological Properties of Mo-S-N Solid Lubricant Coatings**, ***Tomáš Hudec***, University of Southampton, UK*; M Mikula, L Satrapinskyy, T Roch, M Truchlý,* Comenius University in Bratislava, Slovakia*; P Švec Jr.,* Slovak Academy of Sciences, Bratislava, Slovakia*; T Huminiuc, T Polcar,* University of Southampton, UK

Self-lubricant thin solid films produced by physical vapour deposition (PVD) techniques represent modern approach to reduce friction in highly demanding situations where traditional liquid lubricants cause problems (environmental, excessive costs, frequent maintenance) or cannot be used at all (vacuum, extremely high/low temperatures and contact pressures). Transition metal dichalcogenides (TMDs), especially molybdenum disulphide (MoS_2), are the most known and applied solid lubricant coatings; however, its use is limited by environmental sensitivity and low hardness. To improve mechanical and tribological properties, we doped MoS_2 coating with nitrogen.

Mo-S-N solid lubricant films were deposited by pulsed d. c. High Target Utilisation Sputtering (HiTUS) in Ar + N_2 atmosphere. The effect of deposition parameters on chemical composition, structure, mechanical and tribological properties of MoS_x and Mo-S-N coatings was studied; films with the most promising properties have been selected for tribological testing. MoS_x films with S/Mo ratio 1.6 exhibited the coefficient of frictions (COFs) in humid air 0.12 and 0.05 for loads 2 and 15 N, respectively. Mo-S-N films were prepared with nitrogen content in a range of 19 to 50 at., whereas S/Mo ratio varied from 1.2 to 0.4. Mo-S-N films were amorphous or nanostructured with nanograins of molybdenum disulphide. Hardness increased with N doping up to 14 GPa for film with the highest nitrogen content. Friction behaviour in humid air was evaluated using a ball-on-disk tribometer. Globally, the doping with N resulted in hardness in Mo–S–N films one order of magnitude higher than in an undoped one, keeping the friction coefficient at the same level or even lower. These coatings showed remarkable friction coefficients in humid air from 0.18 to 0.06 with loads from 2 to 15 N, respectively. The excellent friction properties were attributed to the formation of a thin molybdenum disulphide tribofilm on the top of the wear track of the film and on the counterpart surface. HiTUS represents a very promising way of depositing thin coatings on the thermally sensitive substrates (e.g. bearing steel) with desired properties.

8:40am **E1-3-FrM-3 Superlubricity with Carbon Coatings Lubricated by Organic Friction Modifiers**, ***Michael Moseler***, Fraunhofer IWM, Germany **INVITED**

Superlubricity of tetrahedral amorphous carbon (ta-C) coatings lubricated with unsaturated organic friction modifiers or glycerol is a well-known phenomenon, but the underlying mechanisms remain elusive. Here, combined experiments and simulations unveil a universal tribochemical mechanism leading to superlubricity of ta-C/ta-C tribopairs. Pin-on-disc sliding experiments show that ultra- and superlow friction with negligible wear can be achieved by lubrication with unsaturated fatty acids or glycerol, but not with saturated fatty acids and hydrocarbons. Atomistic simulations reveal that, due to the simultaneous presence of two reactive centers (carboxylic group and C=C double bond), unsaturated fatty acids can concurrently chemisorb on both ta-C surfaces and bridge the tribogap. Sliding-induced mechanical strain triggers a cascade of molecular fragmentation reactions releasing passivating hydroxyl, keto, epoxy, hydrogen and olefinic groups. Similarly, glycerol's three hydroxyl groups react simultaneously with both ta-C surfaces, causing the molecule's complete mechano-chemical fragmentation and formation of aromatic passivation layers with superlow friction.

9:20am **E1-3-FrM-5 Multipass and Reciprocating Microwear Study of TiN Based Films**, ***Roberto Carlos Vega-Morón***, Instituto Politecnico Nacional Grupo Ingeniería de Superficies, Mexico, México*; D Melo-Máximo,* Tecnologico de Monterrey-CEM, México*; G Rodríguez-Castro,* Instituto Politecnico Nacional, Grupo Ingenieria de Superficies, Mexico, México*; J Oseguera-Peña,* Tecnologico de Monterrey-CEM, Mexico, México*; A Bahrami,* Institute for Metallic Materials, Leibniz-Institute for Solid State and Materials Research Dresden, Germany*; S Muhl,* Instituto de Investigaciones en Materiales-UNAM, México

Titanium nitride-based films were deposited on AISI 316L steel by D.C. unbalanced magnetron sputtering. Adhesion and wear resistance at the micrometric range of the films were studied by changing the gas mixture ratio and the temperature of the substrate during the deposition process. Scanning electronic microscope (SEM), elemental analysis (EDS) and X-Ray diffraction (XRD) were carried out to investigate films physico-chemical characteristics. Also, the examination of topography was conducted by atomic force microscopy (AFM). Mechanical properties were studied by nanoindentation test. Scratch tests were performed with a chrome steel ball (1 mm of diameter) on a 3 mm scratch track and the critical loads were estimated. Additionally, reciprocating microwear and multipass sliding tests were conducted at 0.5 and 1 N using an alumina ball (3 mm of diameter) as counterpart. The coefficient of friction behavior was analyzed and the identification of damage mechanisms were conducted by SEM and optical profilometry.

9:40am **E1-3-FrM-6 Correlation Between Wear Resistance of Ti/TiN Based Films and Deposition Temperature**, ***Fernanda Toledo-Romo***, *R Vega-Morón,* Instituto Politecnico Nacional, Grupo Ingenieria de Superficies, México*; G Rodríguez-Castro,* Instituto Politecnico Nacional, Grupo Ingenieria de Superficies, Mexico, México*; D Melo-Máximo, J Oseguera-Peña, L Melo-Máximo,* Tecnologico de Monterrey-CEM, México*; V Araujo-Monsalvo,* Laboratorio de Biomecánica, Instituto Nacional de Rehabilitación "Luis Guillermo Ibarra Ibarra", México

Ti/TiN bilayer films deposited on AISI 316L by D.C. unbalanced magnetron sputtering were investigated. The mechanical properties, adhesion and wear resistance of Ti/TiN films were evaluated according to the temperature of the substrate during the deposition process. Four temperatures were used for the study, these were: at room temperature, 80, 120 and 200 ° C. The power and gas mixture ratio during the deposition process remained constant. The bilayer system optical inspection was carried out by scanning electronic microscopy (SEM) and the physico-chemical characterization was performed by energy dispersion spectroscopy (EDS) and X-ray diffraction (XRD). Hardness and Young's modulus were determined by instrumented indentation. Scratch tests were performed to evaluate adhesion using a Rockwell C indenter and loads of up to 100 N. Critical loads (Lc) were estimated based on optical microscope observations of the scratch tracks. The wear coefficients of TiN and Ti formed on 316L steel were evaluated by a micro- abrasion tester using SiC particles dissolved in deionized water as abrasive slurry. The wear

coefficients were obtained by relating the Archard law and the wear area (obtained by optical profilometry).

10:00am **E1-3-FrM-7 Microstructure Evolution and Deposition Parameter Control on Sputtering MoSiN Coating**, ***Yu-Cheng Liu***, *Z Lin, S Wang, F Wu,* National United University, Taiwan

Transition mental nitride, TMN, coating due to its excellent surface and mechanical characteristics, was applied in surface finishing, decoration, and protective coating. In present study, the molybdenum silicon nitride, MoSiN, films were produced by RF magnetron sputtering technique for protective application. Microstructure evolution and composition variation were found for the MoSiN coating due to the change of the input power and gas flow ratio during the manufacturing process. The effect of input power control on microstructure evolution and indentation cracking behavior were analyzed. When input powers on Si and Mo were fixed at 105W and 135W, respective, the Si/MoSi contents varied from 0.27 to 0.44 when Ar/N_2 flow changed from 18/2 to 10/10. The microstructure possessed a featureless structure as a high content Si was incorporated. Hardness, Young's modulus, abrasion characteristics of the MoSiN monolayer films were further investigated and discussed.

10:20am **E1-3-FrM-8 Influence of Ag Content on the Tribological and Oxidation Behaviour of TISIN(AG) Thin Films Deposited by HIPIMS**, ***Diogo Cavaleiro***, *F Fernandes, S Carvalho,* University of Minho, Portugal*; A Cavaleiro,* University of Coimbra, Portugal

Titanium alloys are one of the most common materials used in several important industries (aerospace, automotive, etc.) due to its multiple excellent properties. Nonetheless, they are also known as a "difficult-to-machine" material, leading to the premature wear and/or failure of the machining tools and consequently to the increase of the production costs. Self-lubricating coatings (highly oxidation resistant coatings alloyed with a lubricious element) are one of the most promising solutions to overcome this problem. The main challenge nowadays in these type of coatings is to control the diffusion of the lubricious element to the surface. Here, we propose to control the diffusion of silver, using the TiSiN system deposited as nanocomposite structure. Si-N matrix of this coating system is well known to have diffusion barrier properties which with proper tailoring of the structure, could avoid the lubricious agent diffusion. This work reports the influence of Ag additions on the properties of TiSiN(Ag) films deposited by high power impulse magnetron sputtering- HiPIMS. All of the coatings displayed a fcc NaCl-type crystalline structure. Silver addition to the TiSiN coating significantly lowers the TiN crystallites size however, grain size of Ag containing coatings was independent of the coatings chemical composition. Mechanical properties of the coatings deteriorated with the increasing silver content. Ag additions decreases the oxidation behavior of films, however it improves their tribological performance.

10:40am **E1-3-FrM-9 Wear Resistance of Titanium Oxynitride Coatings as a Function of the Relative Humidity**, *C Rojo-Blanco,* IIM-UNAM, Mexico*;* ***Stephen Muhl***, Instituto de Investigaciones en Materiales-UNAM, México

For this study we used titanium oxynitride thin films because of their many uses as coatings in biological, aeronautics, automotive applications. Each application has its own environment with different conditions that can influence the wear of the films. These conditions can involve physical (applied force and temperature, etc.) or chemical (acid, basic, relative humidity, etc.) factors.

The five groups of titanium oxynitride coated samples, with different oxygen to nitrogen ratios, were deposited by RF reactive sputtering on to stainless steel substrates. To analyze the wear we employed the reciprocating sliding test, one of the most common tests. With this technique we could observe the change of the coefficient of friction during the wear process, and subsequently measured the wear volume and study the wear track. In order to control the relative humidity surrounding the point of contact between the deposited film and the counter-body (alumina) we modified our standard reciprocating sliding test machine to include an enclosure connected to the gas flow from a humidity generator. In this way we measured the variation of the wear, using an optical profilometer, as a function of the relative humidity for each group of oxynitride coatings.

11:00am **E1-3-FrM-10 Thermo-mechanical/chemical Contact Behavior of DLC Film under Molecularly Thin Lubricants**, ***Shahriar Mufid Rahman***, Texas Tech University, USA*; J Song,* Molex. USA, USA*; C Yeo,* Texas Tech University, USA

Diamond like carbon (DLC) has been widely used as a surface protective coating due to its outstanding tribological performance. When a DLC coating is required to sustain high speed surface contact at hot/wet condition, its surface is susceptible to critical damage by mechanical and chemical degradation of carbon atoms. In this study, the thermo-mechanical/chemical contact behavior of DLC film under molecularly thin lubricants is investigated through molecular dynamics (MD) simulations. Three different designs of PFPE lubricants (i.e., D4OH, Z-tetraol and ZTMD) are applied onto amorphous DLC film. Under the high-speed sliding contact with an asperity made of diamond, the friction and wear of DLC film is quantitatively measured and compared. From MD simulation results, it could be found that all three lubricants significantly improved the tribological performance of DLC film, and the lubricants with higher molecular weight made further improvements. It is expected that the research outcome can provide more physical insight into the tribological performance of DLC film and PFPE lubricants, which can deliver their key design rules to achieve the long-term reliability of a system.

11:20am **E1-3-FrM-11 Investigation of the Wear Resistance of TiN/TiAlN, CrN/TiAlN and CrAlN/TiAlN Double Layer Coated Stainless Steel at Elevated Temperatures**, ***Akeem Adesina***, *A Sorour,* King Fahd University of Petroleum and Minerals, Saudi Arabia

TiAlN coating is now widely being used as protective coatings against wear and abrasion in turbomachinery, cutting tools and aerospace applications. This is due to its superior mechanical and tribological properties at both low and high temperatures over commonly used TiN coating. However, increasing demands on hard coatings due to increased productivity, new tool applications such as high-speed cutting, dry cutting and/or extreme operating environment have necessitated the need for improved coating performance. Coating architecture, microstructural and compositional modification, as well as advanced deposition technologies, are among methods currently being researched to further improve properties of TiAlN and other hard coatings. The use of an interlayer coating is well known to improve adhesion, corrosion and wear resistance properties. Several efforts are being tailored in order to improve the performance efficiency of TiAlN at elevated temperatures through the use of layers and multi-layered deposits.

This study is aimed at investigating the wear resistance and the effect of TiN, CrN and CrAlN as interlayers for TiAlN at elevated temperatures. The wear behavior of these double layer coatings will be evaluated under reciprocating wear test configuration at room temperature, 250 and 500 °C and compared to the monolayer TiAlN coating (without interlayer) to reveal the role of the interlayer coatings. An attempt will be made to investigate both surface and subsurface damages during wear. 3D optical profilometer, scanning electron microscope (FE-SEM) and energy dispersion spectroscopy (EDS) will be utilized to understand the wear damages and underlying mechanisms. The structural and mechanical characterization of the coatings analyzed using X-ray diffraction (XRD) technique and microindentation, respectively, will also be examined and discussed in light of the wear behavior.

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