Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room San Diego - Session E2-1-TuM

Mechanical Properties and Adhesion I

Moderators: Megan J. Cordill, Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, **Ming-Tzer Lin**, National Chung Hsing University & Chaoyang University of Technology

8:00am **E2-1-TuM-1 Indentation Behavior of Metal-Ceramic Multilayer Coatings: Modeling vs. Experiment***, **Yu-Lin Shen,*** University of New Mexico, USA **INVITED**

Thin films consisting of alternating metal and ceramic layers are an exciting subset of materials with many promising attributes. This presentation highlights our recent studies on mechanical characterization of such coatings using nanoindentation. We focus on aluminum (Al)/silicon carbide (SiC) nanolayers, which serves as a model system for investigating the constraining effect due to the highly mismatched mechanical properties of the constituents. How this structural heterogeneity responds to nanoindentation is a current a subject of active research. The development of complex deformation patterns underneath the indentation, dictated by the structural heterogeneity, can lead to various forms of local damage. Our studies focus on the employment of numerical finite element modeling to corroborate with experimental observations as well as to extract meaningful constitutive properties. Special attention is given to the analyses of (i) plastic deformation in the metal layers, (ii) cyclic indentation response and composite modulus measurement, (iii) indentation-induced delamination, and (iv) indentation-induced shear band formation.

8:40am **E2-1-TuM-3 Indentation Induced Delamination for Adhesion Measurements***, **Megan J. Cordill,** A Kleinbichler,* Erich Schmid Institute of Materials Science, Austria

Silicon nitride (Si_3N_4) is a frequently used passivation layer as well as an ion barrier in microelectronic devices. Its most outstanding properties are high fracture toughness and thermal stability, but in order to have a reliable device the adhesion to other thin films is of great importance. Qualitative tests like tape tests have shown that the adhesion of the brittle interface of Si_3N_4 and silicon glass (BPSG) is rather poor. In order to determine a quantitative measure of the adhesion of Si_3N_4 to BPSG other techniques such as nanoindentation are necessary. Indentation induces well-defined areas of delamination at the Si_3N_4-BPSG interface only when used in conjunction with a stressed overlayer of WTi. In this film system, the stressed overlayer helps the underlying Si_3N_4 film to buckle and supports the delaminated, brittle Si3N4 film from spalling from the substrate. Utilizing the delaminated areas and well established methods the adhesion of brittle thin films can be determined, which could not be measured before.

9:00am **E2-1-TuM-4 Intrinsic Stress in Polycrystalline Film: An Atomistic View***, **Enrique Vasco,*** Instituto de Ciencia de Materiales de Madrid, Spanish National Research Council (CSIC), Spain*; D Franco,* Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain*; E Michel, C Polop,* Departamento de Física de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain

Most of the current applications based on films and coatings use continuous and compact polycrystalline films. They are easy to produce and integrate in many devices, cost-effective and suitable for common applications. However, their reliability suffers as the applications demand more resources, intensive use of medium properties or nonstandard working conditions. These limitations are due to the heterogeneous structure of the polycrystalline films, which are made up of misorientated grains separated by boundaries and other defects. Where the crystal lattice of the films has defects, a local field of intrinsic stress is generated. This stress field, which is reversible and cumulative with the working conditions, determines the short-range properties of the films and shortens the lifespan of devices.

The evolution of the intrinsic stress during the preparation of polycrystalline films has been investigated over decades. Nowadays, it is well known that the continuous compact films grow under compression, whose strength is closely linked with the density of grain boundaries (GB). However, the origin of the compression has not been clarified yet despite many models have been proposed. Recently, we measured the local distribution of residual intrinsic stress in polycrystalline films using a pioneering method[1]of nanoscale stress mapping based on AFM. Our results[2] demonstrated that, at odds with expectations, compression is not generated inside GBs, but at the edges of gaps where the boundaries intercept the surface. We report now a “definitive” model[2,3], wherein the compression is caused by Mullins-type surface diffusion towards the GBs, which generates a kinetic surface profile different from the equilibrium profile predicted by Laplace-Young. Where the curvatures of both profiles differ (mainly, at the edges of gaps where diffusing atoms accumulate), the intrinsic compression rises in the form of Laplace pressure. Our model[3] addresses successfully all the major evidences reported so far regarding the behavior of stress with experimental conditions. However, owing to the mesoscopic nature of our model, it is difficult to correlate it with atomistic processes that provide a physical vision (rather than mathematical one) of the phenomenon. In this work, we update our model in atomistic terms, namely, we address the origin and behavior of the intrinsic compression from the density of surface species (i.e., monomers and steps) and random walk diffusion with aggregation/nucleation leading to step-flow/second-nucleation growths.

1) C. Polop et al., Nanoscale **9**, 13938 (2017)

2) E. Vasco et al., PRL **119**, 256102 (2017)

3) E. Vasco et al., PRB 98, 195428 (2018)

9:20am **E2-1-TuM-5 Development of a Methodology for Measuring the Elastic Constants of Anisotropic Coatings Using Impulse Excitation Technique***, **Elia Zgheib,*** University of Technology of Troyes (UTT) and Lebanese University (UL), France*; M Slim, A Alhussein,* University of Technology of Troyes (UTT), France*; K Khalil,* Lebanese University (UL), Lebanon*; M Francois,* University of Technology of Troyes (UTT), France

New processes for obtaining advanced materials, in the form of coatings, are developing more and more to meet the socio-economic and the environmental needs. Coatings, as protective layers, improve the surface properties of a material. For example, in biomedical, elastic properties are must to be considered for the good insertion of the prostheses into the bone tissues. Thus, the deposit of Micro metric and/or Nano metric layers to obtain gradient functional materials is a promising approach for achieving impedance matching or reduction of stress concentrations on structures, such as prostheses or implants.

The project is part of the developments of Impulse Excitation Technique (IET) measuring constants of elasticity of thin layers [1, 2]. The IET is based on the analysis of vibrational frequencies created by an impact on a specimen. In this project, deposition will be developed using low-pressure process: PVD (Physical Vapor Deposition); and the parameters influencing the elasticity of the coatings will be identified. In the literature and for a designed anisotropic coating, no technique is available to go back to the values of the elastic constants of each layer and stack. This difficulty motivates the researcher to innovate methods and characterizations. What the project proposes is developing an inverse method using a multilayer model and the global analysis of vibration modes obtained by IET.

The methodology being used is a multi-scale approach to correlate the microstructural state of the coating and its resulting properties. The objectives that will be achieved rely on the development of IET measurement technique for mono and multi anisotropic coatings, by understanding the link between the parameters of elaboration, the physical-chemical properties, the microstructures and the elastic constants of the materials.

Keywords: Coatings, Elastic constants, Anisotropy, Multilayers, Impulse Excitation Technique, PVD.

Acknowledgements: The authors would like to thank the co-founders of CERA project: The European Union (Fond Européen de Développement Régional)

References:

[1] M.F. Slim, A. Alhussein, F. Sanchette, B. Guelorget, M. François, A new enhanced formulation to determine Young's and shear moduli of thin films by means of Impulse Excitation Technique, Thin solid films, 2017.

[2] M.F. Slim, A. Alhussein, A. Billard, F. Sanchette, M. François, On the determination of Young’s modulus of thin films with Impulse Excitation Technique, Journal of Materials Research, 2016.

Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room San Diego - Session E2-2-TuA

Mechanical Properties and Adhesion II

Moderators: Megan J. Cordill, Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, **Ming-Tzer Lin**, National Chung Hsing University & Chaoyang University of Technology

2:00pm **E2-2-TuA-2 Mechanical Behavior Study of 50 nm-thick Thin Film of Gold Single Crystal with In situ X-ray Pole Figures Measurements*, Pierre-Olivier Renault,*** Université de Poitiers, France*; J Drieu La Rochelle, P Godard, M Drouet, J Nicolai, M Beaufort,* University of Poitiers, France*; D Thiaudière, C Mocuta,* SOLEIL Synchrotron, France

For a few years, thanks to the development of mechanical tests on nanometer-size objects, the question of how the mechanical plastic behavior of metallic materials change as their characteristic sizes are reduced down to nanometer range has attracted significant interest. In addition to slip by dislocation glide, deformation twinning is one of the plastic deformation mechanisms in metallic crystalline materials. In this way, size-dependent twin propagation behaviors in nanowires such as face-centered cubic metals has been reported in literature.

In this work, the mechanical behavior of gold single crystal is studied thanks to in situ pole figures measurements during controlled biaxial loadings. The gold thin film 50 nm thick is deposited on NaCl single crystal by physical vapor deposition technique at 400°C. The film is then transfered on a polyimide cruciform substrate to be deformed on a biaxial tensile tester in situ during synchrotron x-ray measurements. The as-deposited gold single crystal contains a given amount of small twins. The twins are rather narrow and small, i.e. they have a thickness of about 10 nm and a size of about 50-100 nm.

In the presentation, the first results obtained on in situ uniaxial applied deformation in the [110] direction of Au monocrystalline film are reported. The in situ x-ray pole figure measurements show a huge evolution of the intensity of the diffracting pole related to the twins. Hence, the amount of twins is increasing during deformation, either by thickening or growing of the pre-existing twins, either by creating new twins. The twins' volume is quantified as a function of applied deformation.

2:20pm **E2-2-TuA-3 Evaluation of the Mechanical Properties in Antibacterial Multi-layer HA-Ag Coatings Deposited by RF Magnetron Sputtering*, Julian Lenis,*** *M Gómez, F Bolívar,* University of Antioquia, Colombia

The use of osteoconductive coatings such as Hydroxyapatite (HA) in surgical implants is a great alternative in order to improve the acceptance of these devices in the human body. On the other hand, in order to avoid possible problems associated with bacterial infections, which can be generated during the surgical or postoperative procedure, researchers have been developing antibacterial coatings that act locally inhibiting the bio-film formation. One of the strategies that has been adopted to induce these properties is the incorporation of silver (Ag) nano-particles in HA coatings. In the literature it has been found that these coatings exhibit a good antibacterial behavior, however, there are few studies about the mechanical behavior of these systems deposited like multi-layer coatings. Therefore, in the present report the effect of the process parameters such as deposit temperature and substrate-target distance, on the chemical composition, structure, morphology and mechanical properties of multilayer coatings HA-Ag deposited by magnetron sputtering on Ti6Al4V is shown. The characterization of the obtained films was carried out by means of energy dispersive spectroscopy, micro-Raman spectroscopy, scanning electron microscopy, atomic force microscopy and nano indentation tests. A relationship between the target-substrate distance and the chemical composition of the coatings was found, obtaining a decrease in the Ca/P ratio, as function of the decrease between the target and substrates. Additionally, the critical load of the deposited coatings shown an increasing tendency as function of the decrease in the target-substrate distance, whereas for the first level of cohesive failure an inverse behavior was obtained. Furthermore, both mechanical characteristics were improved with the increase of the deposit temperature.

Key words: magnetron sputtering, hydroxyapatite, multi-layer coating, critical load, first level of cohesive failure.

2:40pm **E2-2-TuA-4 Mechanical Deformation in Metal and Ceramic Nano Multilayers*, Andrea Hodge,*** University of Southern California, USA **INVITED**

Nano multilayers (NMs) consist of alternating layers of materials with thicknesses on the order of nanometers and typically display many attractive properties which are attributed to the fact that, as the layer thicknesses decrease, the individual layer behavior changes and the interface volume increases. In general, studies on the mechanical behavior of NMs have been focused mostly on metal systems, followed by metal/ceramic systems and even fewer studies on ceramic multilayers. Thus, the behavior of metallic NMs is well characterized and general trends such as a Hall-Petch type strengthening behavior has been observed for variety of material systems as result of the layered structure. In contrast, for ceramic NMs, the research is limited and overall trends and mechanisms have not been well determined. Furthermore, for NM ceramics, the role of dislocations is limited and therefore the role of the interfaces increase and hold the key to understanding their mechanical behavior.

In this study, we present a comprehensive microstructural evaluation of metal and ceramic multilayers with various layer thicknesses and compositions in order to elucidate on the role of their interfaces during mechanical deformation. Several NM configurations including SiO_2/TiO_2, AlN/SiO_2, AlN/Ag, Cu/Nb, Mo/Au and Hf/Ti will be presented. The role of bilayer thickness and composition is evaluated in both compression and tension using nanoindentation and micro-tensile tests.

4:00pm **E2-2-TuA-8 Deposition of Highly Adhesive Ta Based Thin Films on a Biomedical Grade CoCrMo Alloy*, Jesus Corona-Gomez,*** *Q Yang, Y Li,* University of Saskatchewan, Canada

Tantalum (Ta) based thin films including alpha and beta tantalum, TaN, and Ta doped diamond-like carbon (Ta-DLC) thin films deposited by radio frequency (RF) magnetron sputtering were investigated as potential interlayers to enhance DLC coating adhesion on a biomedical grade CoCrMo alloy. The deposited interlayers and DLC thin films were characterized by X-ray diffraction, Raman spectroscopy, and Rockwell C indentation. The correlation between the adhesion and the structure of interlayers was investigated. The results show that the deposition temperature and bias voltage play an important role in determining the structure and adhesion of the interlayers and thus the adhesion of DLC coatings.

4:20pm **E2-2-TuA-9 DIC on FIB Ring-Core of Thin Films for Depth Sensing Residual Stress Measurement*, Ming-Tzer Lin,*** *W Pan,* National Chung Hsing University, Taiwan*; T Chen, F Cheng,* National Cheng Kung University, Taiwan*; J Huang,* National Tsing Hua University, Taiwan

Reliable measurement and modeling of residual stresses at the micrometer scale is a great challenging task for small-scale structures and nanostructured thin films. Moreover, the specific location on microscale evaluation of residual stress gradients is a very critical issue in the hard coating of thin films. The analysis of the residual strain depth profiles requires detailed knowledge of the in-depth lattice strain function, so the residual stress profile calculation can be carried out in a manner that takes into account the mechanical anisotropy and texture of the materials. The development of a microstructure independent procedure for depth-resolved measurement of residual stress is an issue of strategic interest. Here, we perform a digital correlation (DIC) of the specimen images acquired by incremental focused ion beam (FIB) ring-core drilling with various depth steps. A translation test was performed first to study the applicability of DIC to FIB images, and a proper procedure was established to obtain more accurate results. Next, 2 um thick sputtered Ag and ZrN thin films were used for this measurement. To observe the depth-resolved residual stress profiles of each step on thin film samples, two FIB images of the specimen, one before and one after being drilled, were processed to extract the surface deformation from tiny changes in the FIB images using DIC. This combined with high-resolution in situ SEM imaging of the relaxing surface and a full field strain analysis by digital image correlation (DIC). A parallel residual stress measurement was also performed using a four-circle diffractometer with grazing incidence X-ray diffraction (XRD) $\cos^2\alpha\sin^2\Psi$ method at several azimuthal angles to obtain the average X-ray strain (AXS) and thus the residual stress can be accurately determined and compared.

4:40pm **E2-2-TuA-10 Metallic Glass/Crystalline Nanolayered Coatings with High Nanoscratch Resistance and Damage Tolerance***, M Abboud,* Middle East Technical University, Turkey*; A Motallebzadeh,* Koç University, Turkey*; **Sezer Özerinç**,* Middle East Technical University, Turkey

Metallic glass/crystalline metal nanolayers provide a balanced combination of high hardness and ductility, making them promising materials for wear resistant coating applications. However, there has been no study to date investigating the wear behavior of these materials. In this study, we investigated the nanoscratch behavior of nanolayered CuZr/Zr composed of alternating CuZr metallic glass and nanocrystalline Zr layers.

A magnetron sputterer deposited the 1 µm thick coatings on polished 316 stainless steel substrates. Layer thickness varied in the range 10-100 nm. X-ray diffraction and transmission electron microscopy characterized the microstructure of the coatings and nanoindentation measurements probed the hardness and elastic modulus. A nanoindenter equipped with a sphero-conical diamond tip of 5 µm radius performed nanoscratch measurements on the coatings.

Hardness and elastic modulus of nanolayered coatings do not vary with layer thickness and are close to that of the monolithic metallic glass, about 5.5 GPa, and 105 GPa, respectively. A comparison of nanoscratch residual depths, on the other hand, indicate that monolithic CuZr has higher scratch resistance than the layered samples. Among the nanolayers, CuZr/Zr with 100 nm layer thickness shows the highest scratch resistance, and the resistance diminishes with decreasing layer thickness. All coatings showed considerably smaller penetration depth when compared to uncoated stainless steel demonstrating the superior wear resistance and damage tolerance of the coatings.

A close observation of scratch tracks showed outstanding adhesion and conformity of the coatings to the substrates. The most damage tolerant coating was the CuZr/Zr with 10 nm layers, showing no sign of delamination or fracture at compressive strain levels exceeding 80%. Monolithic CuZr showed local delamination and microfracture at relatively lower strain levels, but without any gross failure.

Although the hardness and elastic modulus of the coatings are virtually the same, the nanoscratch results indicated distinct patterns. We attribute the layer-thickness dependent behavior to the low interfacial shear strength in these layers previously reported in literature. While low interfacial strength does not play a major role in nanoindentation response where plastic strain is mostly perpendicular to the interface, it affects the scratch resistance where shear strain is dominant. Our findings give insight to the behavior of metallic glass/crystalline composites under sliding loading conditions for the first time in the literature, and present a model system for the development of protective coatings suitable for compliant substrates.

5:00pm **E2-2-TuA-11 Coatings Effect On Crack Initiation Behavior Of Ti Alloys***, **Xiaolu Pang**,* University of Science and Technology Beijing, China

Titanium has high strength/weight ratio, stiffness and corrosion properties, but at the same time different kinds of surface treatments are employed due to the poor wear resistance, and surface coating is one of the most popular ones. Since fatigue is one of the most important properties of titanium alloys and fatigue crack initiation period occupy an important position in the fatigue failure process, so the study on coating effect on fatigue crack initiation should play an important role. However, the effect of coatings on fatigue crack initiation of Ti-alloys has not be taken seriously, and the mechanism is not clear. This paper deposited CrAlN and TiN hard coatings by PVD on the surface of TC4 titanium alloy to study the coating effects on fatigue crack initiation and propagation. Hard coatings significantly decreased fatigue properties of TC4, since the 510-530 MPa TC4 fatigue limit was reduced to 315-330 MPa for the CrAlN coated samples. The existence of coatings prevented deformation of the TC4 samples at the beginning of fatigue tests, and had a positive effect on sample deformation in the middle of the fatigue process. For the coated samples, the fatigue crack initiated in the coatings and propagated to the interface, and induced a micro crack at the substrate surface. Then the micro crack propagated into the bulk material and formed the distinct propagation path in the fracture surface. The mechanism of non-propagation fatigue cracks and influence of coating thickness were also studied. A corresponding model is proposed.

Tribology and Mechanical Behavior of Coatings and Engineered Surfaces

Room San Diego - Session E3-WeM

Tribology of Coatings for Automotive and Aerospace Applications

Moderators: John Curry, Sandia National Laboratories, USA, **Christian Greiner**, Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), **Oliver Hunold**, Oerlikon Balzers, Oerlikon Surface Solutions AG

8:00am **E3-WeM-1 Self-assembly of Ultra-high Strength Nanoporous Metals for Multifunctional Coatings and Free-standing Films*, James Pikul,*** University of Pennsylvania, USA*; N Argibay, J Curry,* Sandia National Laboratories, USA*; Z Hsain,* University of Pennsylvania, USA **INVITED**

This talk will describe the fabrication and characterization of nickel-based cellular materials which have the strength of titanium and the density of water. These materials can be made free-standing or as thin film coatings by electroplating metal through self-assembled particles. The gap between self-assembled particles confines the dimension of the metal struts to diameters as small as 17 nm. The nanoscale confinement increases the local yield strengths of the nickel struts to 8 GPa, which exceeds that of bulk nickel by up to 4X. The mechanical properties of this material can be controlled by varying the nanometer-scale geometry, with strength varying over the range 90-880 MPa, modulus varying over the range 5-40 GPa, and density varying over the range 880 – 14500 kg/m^3. In addition to characterizing the mechanical strength of these nickel-based cellular materials, I will discuss their wear performance when the pores are infiltrated with solid lubricants. These materials present a new class of films that can achieve high wear resistance while also maintaining high thermal conductivity, electrical conductivity, or other tailored properties.

8:40am **E3-WeM-3 Elevated Temperature Sliding Wear of PEO-Chameleon Duplex Coating*, Andrey A. Voevodin,*** *A Shirani,* University of North Texas, USA*; A Yerokhin,* The University of Manchester, UK*; A Korenyi-Both,* Tribologix Inc., USA*; D Berman,* University of North Texas, USA*; J Zabinski,* Army Research Laboratory, USA

Plasma electrolytic oxidation (PEO) is an attractive technology for improving wear and corrosion resistance of aluminum and titanium alloys exposed to different temperature and environment.. PEO results in formation of 50-150 micrometer thick hard ceramic (AlSiO and TiSiO) coatings with good adhesion to the substrate and with morphology gradient from a dense region near the substrate interface to a porous outside region [1]. Such properties potentially make a PEO coating an ideal underlying layer for the application of solid lubricants which can be entrapped in outside porous and provide reservoirs for the tribological contact lubrication. In this study we investigate the wear behavior of the PEO –based coatings during sliding in air at elevated temperatures. The PEO produced 11-12 GPa hardness AlSiO and TiSiO coatings are covered with a top layer of an MoS_2-Sb_2O_3-graphite chameleon solid lubricant, the composition of which was previously reported to self-adapt in variable humidity environments resulting in friction and wear reduction [2]. Coupons of aluminum and titanium alloys were coated by the PEO process and then were over-coated by a burnishing process with a MoS_2-Sb_2O_3-graphite chameleon coating to prepare such duplex coating combination. The coated surfaces were then subjected to sliding wear tests against silicon nitride counterparts with variable normal loads (2- 10 N) and temperatures (room to 400 °C). At room temperature, the humid air friction coefficients were of the order of 0.10-0.15, which is typical for graphite lubricant in humid air. However, when the temperature was increased first to 100°C and then up to 400 °C, the coefficient of friction was reduced to about 0.03-0.05 level which was linked with removing the water and promoting lubrication with the MoS2 chameleon coating component. Raman, SEM and cross-sectional FIB/SEM/EDX analyses of the wear tracks were used to investigate the mechanisms of the temperature adaptation and sliding wear performance. The study demonstrate the effectiveness of the PEO-chameleon coating system performance for the sliding wear mitigation and friction reduction.

[1] A.L. Yerokhin et al., Surface and Coatings Technology, 122 (1999) 73.

[2] J.S. Zabinski et al., Tribology Letters, 23 (2006) 155.

9:00am **E3-WeM-4 Formation Mechanisms of Zn, Mo, S and P Containing Reaction Layers on a DLC Coating***, K Bobzin, T Brögelmann, C Kalscheuer,* ***Matthias Thiex,*** Surface Engineering Institute - RWTH Aachen University, Germany

Environmental restrictions on the climate-damaging CO_2 emissions in the field of mobility are increasingly tightened due to political requirements. Thus, there are requirements on saving fossil resources in tribological contacts, e.g., by reducing friction and wear as well as the amounts of additives and lubricants. A successful approach is the application of diamond-like carbon (DLC) coatings on components such as pistons, piston rings and bearings in lubricated tribological contacts due to their significant effects in friction and wear reduction. Lubricants and additives nowadays are designed for tribological steel/steel contacts, whereby the knowledge on tribochemical layer formation on steel surfaces is comprehensive in contrast to the physical-chemical interactions between DLC coatings, lubricants and additives. That is in contradiction to the increasing usage of DLC coated components in tribological applications. Within this study, the formation mechanisms of Zn, Mo, S and P containing reaction layers on a Zr modified DLC coating a–C:H:Zr (ZrC_g) in lubricated tribological DLC/DLC contacts were studied by means of pin-on-disc (PoD) tribometer. Motivated by the loading conditions in applications, the tests were conducted by varying the distances in a range 200 m ≤ s ≤ 5,000 m under boundary and mixed friction conditions at a temperature T = 90 °C and a Hertzian contact pressure p = 1,300 MPa. The synthetic base lubricant poly-alpha-olefin (PAO) was formulated using the anti-wear (AW) and extreme pressure (EP) additive zinc dialkyldithiophosphate (ZnDTP), PAO/ZnDTP, the friction modifier (FM) additive molybdenum dialkyldithiophosphate (MoDTP), PAO/MoDTP, as well as a combined additivation of MoDTP and ZnDTP at a ratio of 1:3, PAO/MoDTP/ZnDTP/1:3. Based on the results of confocal laser scanning microscopy (CLSM), tribochemical layers form inside and at the edge region of the wear track. The chemical and structural formation process can also be influenced by increasing the sliding distance s in PoD tests. Hereby, the thickness of the tribochemical layers increases too. The chemical composition of the tribochemical reaction layers (Zn,Mo,S,P) and molybdenum disulphide (MoS_2) determined by energy-dispersive X-ray spectroscopy (EDX) and Raman spectroscopy differs by changing the additivation and sliding distance s. Similar conclusion can be made considering the structure and texture of the tribochemical reaction layers, which differ significantly in size and appearance for all analyzed tribological contacts. Hereby, the results show the importance of a differentiated consideration of the interaction between DLC coating, lubricant and additive.

9:20am **E3-WeM-5 ta-C Coatings for Tribological Applications***, J Becker,* Oerlikon Balzers Coating Germany GmbH, Germany*; N Beganovic,* ***Astrid Gies****, J Karner,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; J Vetter,* Oerlikon Balzers Coating Germany GmbH, Germany

Diamond Like Carbon (DLC) coatings and in particular the hydrogenated a-C:H coatings are widely used where friction and wear reduction is required. However, a-C:H coatings have a limited thermal stability and start to graphitize at temperatures higher than about 300°C. Depending on the contact pressure, graphitization might even occur at much lower temperatures. In addition, the tribological performance of a-C:H coatings can be negatively influenced by different lubricants and additives.

To overcome the drawbacks of a-C:H coatings hydrogen-free DLC coatings like ta-C and a-C are currently investigated as a possible solution. ta-C shows a significant higher coating hardness than a-C:H coatings and due to the lack of hydrogen a different surface chemistry which results in a different behaviour under lubricants. ta-C is usually deposited by high-energy deposition processes like arc evaporation; the arc evaporation is possible with or without filtering. Inherent to these processes is the generation of coating defects like droplets. A suitable post-treatment is mandatory to reduce the roughness to an acceptable level. High roughness in combination with a high coating hardness would lead to significant counter body wear.

In this work, ta-C coatings were submitted to tribological testing in a wide temperature range (room temperature to 480°C) in dry running conditions under air. Surprisingly the maximum operation temperature in dry running systems was not as high as expected. The results were compared to those obtained in the past for a-C:H coatings [1]. The investigations were completed by Raman measurements for a better understanding of the tribological behavior of the coatings. In addition, we investigated the compatibility of ta-C with different lubricants and additives and compared it to a-C:H.

[1] J. Becker et al., Thermal effects influencing stability and performance of coatings in automotive applications, Surface & Coatings Technology 284 (2015), pp. 166-172

11:00am **E3-WeM-10 Titanium Nitrides Coatings for Hard Chromium Replacement***, **Marjorie Cavarroc,*** Safran Tech, France*; B Giroire, L Teulé-Gay, D Michau, A Poulon-Quintin,* ICMCB, France

High-power impulse magnetron sputtering (HIPIMS or HiPIMS, also known as high-power pulsed magnetron sputtering, HPPMS) is a method for physical vapor deposition of thin films which is based on magnetron sputtering deposition. Very high power densities (of the order of a few $kW\cdot cm^{-2}$) are applied in very short pulses (few tens of microseconds) at low duty cycle (< 10%).

HIPIMS allows reaching a high ionization degree of the sputtered material around several tens of percent versus a few percent for conventional magnetron sputtering. The ionization and dissociation degree increase as a function of the peak cathode power. The limit is determined by the transition of the discharge from glow to arc phase. In the system we used, a continuous voltage is applied to the discharge in order to maintain continuously the plasma and increase its stability.

Work was focused on Titanium Nitride (TiN) deposition on steel coupons. After optimizing parameters for Titanium sputtering, the following parameters were chosen: 1 Pa total pressure, gas mixture 5% N2 diluted in 95% Ar. High power pulses of 20 µs @ 200 Hz were delivered with a voltage comprised between 800V and 900V and a continuous voltage comprised between 90V and 150V. In those conditions, maximum intensities around a few tens of amperes are observed.TiN coatings we obtained exhibit a cubic crystalline structure, with a low film texturation and nanometric crystallites.

Coatings are continuous and fully covering the substrate. TiN morphology and roughness are directly linked to the substrate's ones. Coatings are homogeneous in all the thickness: micro-stress, crystallite size and chemical composition are the same from the surface to the interface with the substrate.

We will present the influence of deposition parameters on the coating microstructure (crystallinity, stoichiometry, grain size and interface). Tribological properties will also be discussed.

11:20am **E3-WeM-11 Tribological Coating Solutions and Lubrication Strategies for Gas Turbine Engines***, **Pantcho Stoyanov,*** Pratt & Whitney, USA

The advancement of durable gas turbine engine components depends heavily on the development of high-performance materials that can withstand extreme environmental and contact conditions (e.g. large temperature ranges, high contact pressures, and continuous bombardment of abrasive particles, all of which degrade the physical properties). In particular, due to the large number of complex contacting and moving mechanical assemblies in the engine, the lifetime of certain structures is limited by the tribological performance of the employed materials and coatings. This talk will provide an overview of tribological solutions and lubrication strategies employed in several sections of gas turbine engines. After a general review of aircraft engine tribology, the talk will focus on tribological coatings and materials used to minimize fretting type of wear. A series of studies on the friction and wear behavior of Ni-based and Co-based superalloys at elevated temperatures will be presented. Emphasis will be placed on the correlation between the third body formation process (e.g. oxide layer formation, transferfilms) and the tribological behavior of the superalloys. This talk will conclude with the future strategies of tribological coating solutions in gas turbine engines.

Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room San Diego - Session E1-4-WeA

Friction, Wear, Lubrication Effects, and Modeling I
Moderators: Nazlim Bagcivan, Schaeffler Technologies GmbH & Co. KG, Germany, **Carsten Gachot**, Vienna University of Technology

2:20pm **E1-4-WeA-2 Surface Characteristics of the Chameleon/PEO Coating after Fretting Wear Tests*, Mengyu Lin,* *A Nemcova,* University of Manchester, UK*; A Voevodin,* University of North Texas, USA*; T Liskiewicz,* University of Leeds, UK*; A Matthews, A Yerokhin,* University of Manchester, UK

A duplex MoS_2/Sb_2O_3/graphite chameleon and PEO coating deposited on 6082 series Al alloy substrate have been established using burnishing process and plasma electrolytic oxidation (PEO) technique, respectively. A series of fretting wear tests were then applied on the surface of the chameleon/PEO coating sample under various amplitudes and environment (ambient humid air or nitrogen atmosphere) with two different counterpart materials. The X-ray diffraction (XRD), nano indentation, scanning electron microscopy (SEM), energy dispersive spectrometer (EDS), laser confocal microscope and Raman spectroscopy were employed to examine the phase composition, nanohardness, surface microstructure, element distribution and 3D surface topographies of the wear scars. It was found that the wear scars on the chameleon coating were mainly composed of MoS_2, Sb_2O_3 and Al_2O_3 phases while the underneath PEO coating was consisted of crystalline α/γ-Al_2O_3 mixtures. This study demonstrated the efficient wear properties enhancement of the chameleon/PEO coating against alumina counterpart by reducing friction coefficient from 0.88-0.92 to 0.07-0.09 in N_2 and 0.58-0.62 to 0.10-0.12 in air . The specific stick sliding (~3 µm amplitude), partial slip (5-10 µm amplitude) and gross slip (>10 µm amplitude) regimes were observed at the fretting wear with the amplitudes increase from 3 µm to 100 µm. The steel counterpart and oxidized atmosphere were proved could seriously affect the performance of the duplex coating, resulted in the mass generation of the metal oxides/hydroxides in the contact region, long penetration micro-cracks in the PEO coating and gradually severely oxidation in the aluminium substrate.

2:40pm **E1-4-WeA-3 Characterization of W Alloyed DLC Coatings Deposited by a Hybrid DC / HIPIMS Magnetron Sputtering Process*, Manuel Evaristo,*** *A Cavaleiro,* SEG-CEMMPRE - University of Coimbra, Portugal

Tribology is a key feature to sustainable and environmental friendly engineering as it is directly related to energy consumption, wear and component failures across all industries. Energy losses worldwide due to friction and wear have a significant impact on the economy, reduction of friction and wear can reduce economic losses by energy saving and increase time between maintenance stops. One of the most efficient way to reach those objectives is modifying the surfaces in contact by means of thin films in dry and lubricated conditions. DLC coatings provide low friction and good wear resistance in dry sliding; however in lubricated conditions the efficiency is not so good due to inertness of the surface. Therefore, to maintain a good performance in both situations, improving the reactivity of the surface, by doping the coating with a metal, is necessary.

W-DLC coatings were deposited in a four magnetron semi-industrial PVD TEER Coatings deposition chamber with HIPIMS and DC power supplies connected to the W target and C/Cr (used for the deposition of the interlayer) targets, respectively. The depositions were set to have a W content close to 10 at. % for all coatings. The coatings were deposited with two peak power levels, high 140 kW and low 55 kW. For both powers the substrate bias voltage was varied from 0 to -110V. The mechanical properties are influenced by both peak power and bias voltage with the lowest value of 9.7 GPa achieved for the lower peak power and 0 substrate bias and the highest of 14.1 GPa for the higher peak power and 110 V of substrate bias. A coating deposited in a reactive atmosphere (Ar +CH_4) with the latter conditions, with same W content, also showed a similar hardness value 14.9 GPa. The adhesion of the coatings was similar for all coatings tested. The XRD analysis showed typical diffraction patterns of an amorphous structure without visible differences among the coatings. However, both bias and peak power influenced the coatings morphology, with a more compactness columnar aspect with their increase. In the case of the coatings deposited in a reactive atmosphere, a dense and featureless morphology was produced.

Two coatings were selected for the tribological characterization, the ones deposited high peak power and -110V substrate bias, with and without CH4 as reactive gas. The coatings were tested in different conditions with wear rates and coefficient of friction values lower than 0.15×10^{-6} mm^3/Nm and 0.25 respectively.

3:40pm **E1-4-WeA-6 Analysis of Tribomechanical Behavior of Low-Temperature Plasma Blued Tool Steels*, Fernando Santiago,*** ITESM Estado de México, Mexico*; R Meza,* Termoinnova, S.A. de C.V., Mexico*; J Oseguera-Peña,* Tecnológico de Monterrey, México

The tribomechanical behavior of tool steels AISI 4140T and AISI 8620 steel treated by the novel low-temperature plasma blued (LTPB) process. An amorphous solid carbon film (Diamond-like Carbon, DLC) layer is obtained using an atmosphere of methane (CH_4) and molecular hydrogen (H_2) at low-temperature and a short period of time. The microstructure of treated samples was characterized using XPS spectroscopy, Raman spectroscopy, and X-ray diffraction, and the compound layer thickness was measured by optical microscopy. Raman spectroscopy finds D and G bands, and XPS spectroscopy shows a mixture of sp2 and sp3 hybridized bonds of a typical DLC coating. Vickers microhardness profiles were correlated with a reduction of friction coefficient in the treated samples. Wear test was performed on a pin-on-disc tribometer in dry-sliding conditions using a counter-face of WC-Co ball. Wear tracks on the ball and surface of the treated sample were analyzed by optical micrograph and SEM.

Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room San Diego - Session E1-1-ThM

Friction, Wear, Lubrication Effects, and Modeling II

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

8:40am **E1-1-ThM-3 Sliding Wear Resistance of Nickel Boride Layers on Inconel 718 Superalloy**, *I Campos-Silva,* Instituto Politecnico Nacional Grupo Ingeniería de Superficies, México*; **Alan Daniel Contla-Pacheco,*** Instituto Politecnico Nacional, Grupo Ingeniería de Superficies, México*; U Figueroa-Lopez,* Tecnologico de Monterrey-CEM, Mexico*; J Martinez-Trinidad, A Ruiz-Rios, M Ortega-Aviles,* Instituto Politecnico Nacional Grupo Ingeniería de Superficies, México

New results about the wear resistance of nickel boride layers under dry sliding conditions were estimated in this work. For this purpose, an Inconel 718 superalloy was borided using the powder-pack process at two different conditions to estimate the influence of the nickel boride layer thicknesses on the sliding wear resistance. The first condition was at 1173 K with 2 h of exposure (B1), while 1223 K with 6 h of exposure was used for the second condition (B2). A flat-uniform nickel boride layer was developed at the surface of the borided Inconel 718 superalloy with a layer thicknesses ranged between 19 to 50 microns according to the boriding conditions. The microstructure of the nickel boride layer consisted of a mixture of Ni_4B_3, Ni_2B and Ni_3B phases with a presence of a diffusion zone beneath the layers. Otherwise, the indentation properties such as hardness, Young's modulus and the distribution of residual stresses across the boride layer-substrate system were estimated for both boriding conditions.

The sliding wear tests were performed on both boriding conditions and over the untreated material (Inconel 718 superalloy), using a ball-on-flat configuration comprised with an alumina ball of 6 mm diameter as a counterpart, in which a constant load of 20 N was employed with different sliding distances between 50 to 200 m. In addition, during the wear tests, the friction coefficient was monitored for the overall set of experimental conditions.

As it expected, the presence of the nickel boride layers at the surface of the Inconel 718 superalloy enhanced the wear resistance than that of the untreated material. However, for the B2 condition, an increase of the nickel boride layer thickness produced a more wear-resistant layer, in which the values of the wear rate remained constant for the entire set of sliding distances, in contrast with the results estimated for the B1 condition. Finally, the failure mechanisms developed over the surface of the wear tracks for the borided Inconel 718 superalloys (B1 and B2 conditions), and untreated material were discussed and correlated as a function of the friction coefficients and the mechanical properties estimated by indentation tests.

9:00am **E1-1-ThM-4 A Study of the Wear Mechanism of PTFE: The Effects of Temperature and Environment on its Mechanical and Tribological Properties**, ***Vilayvone Saisnith,*** *V Fridrici,* Ecole Centrale de Lyon, LTDS - Université de Lyon, France

Polytetrafluoroethylene (PTFE) coatings are widely employed in various industrial applications due to their low coefficient of friction, low surface energy, good chemical and high temperature resistances. However, PTFE exhibits relatively weak mechanical strength and its wear resistance (particularly in abrasion conditions) has been a critical issue which needs to be understood and to be overcome. In the present work, we set up a methodology to obtain a measure of the durability of PTFE coatings. Experiments to study the effect of both temperature (from room temperature to 180°C) and environment (dry, in water and in an oil) on the mechanical and tribological properties of PTFE have been carried out. The interactions between temperature and environment are also investigated. Scanning Electron Microscopy (SEM) was used to investigate the worn surfaces and debris and thus understand the wear mechanisms under various conditions. As expected, experimental results showed that the tribological resistance of PTFE significantly decreases with increase in temperature. In addition, the coefficient of friction exhibits no significant difference as a function of the environment. The morphological study of wear debris observed after tests at different temperatures and the measurements of mechanical properties of the coating by nano-indentation at different temperatures helped us understand the various wear mechanisms occurring during these tests. In particular, the higher wear observed in an oil environment could be attributed to a different tribological behavior of the transfer film on the abrasive counterbody, with its ease of formation and regeneration.

9:20am **E1-1-ThM-5 Harness Intrinsic Friction in Transition Metal Dichalcogenides**, ***Antonio Cammarata,*** Czech Technical University in Prague, Czech Republic*; T Polcar,* University of Southampton, UK

One of the main difficulties in understanding and predicting frictional response is the intrinsic complexity of highly non-equilibrium processes in any tribological contact, which include breaking and formation of multiple interatomic bonds between surfaces in relative motion. Moreover, under tribological conditions, local charge accumulation may take place and produce a tribological response different than that of the corresponding neutral structure.

To understand the physical nature of the microscopic mechanism of friction and design new tribologic materials, we conducted a systematic quantum mechanic investigation at the atomic scale on prototypical Transition Metal Dichalcogenides at different charge content and applied external load. We combined group theoretical analysis and phonon band structure calculations with the characterisation of the electronic features using non-standard methods such us orbital polarization and the recently formulated bond covalency and cophonicity analyses. We proposed a phonon-mode based method, named Normal-Modes Transition Approximation, to identify possible sliding paths from only the analysis of the phonon modes of the stable geometry and to tune the corresponding sliding energy barriers. We formulated guidelines on how to engineer intrinsic friction at nanoscale, and finally applied them to design a new Ti-doped MoS_2 phase with expected improved tribological properties.

Finally, thanks to the general formulation of our approaches, the present outcomes can be promptly used to finely tune physical properties for the design of new materials with diverse applications beyond tribology such as tuning of Metal-Insulator transitions, dielectric response, Second Harmonic Generation, phase matchability, and ionic conduction among others.

9:40am **E1-1-ThM-6 Static Friction at High Temperature: from Methodology to Severe-Service Valve Application**, ***Thomas Schmitt,*** *J Schmitt,* Polytechnique Montréal, Canada*; É Bousser,* École Polytechnique de Montréal, Canada*; M Azzi,* Tricomat, Canada*; F Khelfaoui, V Najarian, L Vernhes,* Velan*; J Klemberg-Sapieha,* Polytechnique Montréal, Canada

An international effort is being made to increase the thermodynamic efficiency of thermal power plants up to 50%. To achieve this goal, the temperature and pressure of the steam powering the turbines must be increased up to 760°C and 35 MPa. For such grueling application, Metal-Seated Ball Valves are usually the preferred solution for safety valves. Their sealing surfaces being inherently protected in both open and closed positions, they can be exposed to long periods of immobility in harsh environments. Consequently, new materials are being developed to withstand this new application, driving the development of new equipment and methodologies to characterize these materials under severe conditions.

To investigate this specific static contact, a new tribometer has been developed to measure the coefficient of static friction (μ_s) between a pin and a plane up to a 800°C and after several hours of immobility. In parallel, a methodology was established to simulate the contact condition in a valve consisting of Stellite 6 and hard chrome plating. The evolution of the static coefficient of friction was measured according to three parameters: the contact pressure (P_c), the temperature (T_c) and the holding time (t_c). The microstructure, chemical composition, and topography of the contact was then analyzed.

The study revealed that μ_s was not affected by the contact condition at RT. However, at higher temperatures, the coefficient of static friction depended on both contact pressure and holding time. Particularly, at 800°C, the friction behavior was characterized by an increase in μ_s as a function of holding time up to values greater than 1. In addition, much more pronounced adhesive damage was observed compared to other testing temperatures. The above observations were attributed to the evolution of the contact as a function of the testing conditions. In particular, the formation of a mixed oxide inside the contact seemed to have a major influence on the tribological response of the system. Finally, an adhesion mechanism was proposed to explain the origin of the evolution of the static coefficient of friction.

10:00am **E1-1-ThM-7 Coating Development, Characterization and Application-oriented Tests**, ***Lars Pleth Nielsen**, K Almtoft, B Christensen, S Louring,* Danish Technological Institute, Denmark*; H Ronkainen, T Hakala,* VTT Technical Research Centre of Finland, Finland*; D Drees,* FALEX Tribology, Belgium **INVITED**

Developing new coatings and bringing them out of the R&D phase into actual applications is not an easy task. The presentation illustrates how we have developed new coatings based on reactive sputtering processes utilizing different plasma techniques, HiPIMS, pulsed DC and DC magnetron sputtering. The HiPIMS platform was used to develop a very hard TiB_2 coating characterized by having a low residual stress level. Pulsed DC magnetron sputtering was used to deposit a stable 50 µm thick amorphous Al_2O_3 coating for CERN's next generation superconducting magnets. Finally, DC magnetron sputtering was used to deposit different types of low friction carbon-based coatings tailored for different applications such as a low-friction coating for dental application and a Si-containing a-C:H:Si coating revealing increased hardness and improved temperature stability as compared to a-C:H.

The developed coatings were characterized by SEM, nanoindentation, RBS, XPS, GDOES, XRD, etc. The presentation will provide examples of model tests including different types of wear tests as e.g. pin-on-disk, reciprocal sliding tests, scratch testing as well as more application-oriented tests that might be more useful when bringing new coatings into industrial applications.

Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room San Diego - Session E1-2-ThA
Friction, Wear, Lubrication Effects, and Modeling III

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

1:40pm **E1-2-ThA-2 Exploring the Nanomechanical Properties of Transition Metal Dichalcogenides using Density Functional Theory***, **Benjamin Irving**, P Nicolini,* Czech Technical University in Prague, Czech Republic*; T Polcar,* University of Southampton, UK

Low-dimensional materials have recently attracted immense interest due to their fascinating physical properties and potential for application in diverse fields such as (opto)electronics, energy harvesting and dry lubrication. Transition metal dichalcogenides (TMDs), of general form MX_2 (M = Mo, W; X = S, Se, Te), are posited as being some of the best solid-state lubricants currently available. They exhibit a lamellar structure in which covalently-bonded MX_2 layers are held together by weak van der Waals forces, which, together with very low ideal shear strengths (i.e., the maximum load applied parallel to the face of the material that can be resisted prior to the onset of sliding) render them suitable for use in the mitigation of friction. Our extensive density functional calculations highlight the dependence of important nanomechanical properties of TMDs on their chemical composition and bilayer orientation (sliding direction); in particular, our calculations underscore the intrinsic relationship between incommensurate layers and superlubricity.[1] Our latest calculations have focused on TMD-based van der Waals heterostructures (e.g. WS_2 sliding on MoS_2), with the aim of formalizing the relationship between fundamental quantum chemical parameters of the constituent elements and the nanomechanical properties of the material. Ultimately, we wish to improve the predictive capabilities of *in silico* methods during the material design process.

[1] B. Irving, P. Nicolini and T. Polcar, *Nanoscale*, 2017, 9, 5597-5607

2:00pm **E1-2-ThA-3 Mechanics, Materials, and Design Problems in Medical Device Technology and Information Storage***, **Frank E. Talke,*** University of California, San Diego, USA **INVITED**

Current research in medical device technology and information storage at the Center for Memory and Recording Research will be discussed with emphasis on mechanics and materials issues.

In the area of medical device technology, the design of a minaturized pressure sensor for implantation in the eye will be discussed to help in the understanding and treatment of glaucoma. The sensor is a passive devise, based on interferometry, and does not require a power source to be implanted in the eye. Another materials related topic is concerned with the design and development of a 3-d printed disposable endoscope to avoid spread of antibiotic resistant superbugs, a serious medical infection and contamination problem. Materials and manufacturing isues will be discussed. In the area of information storage on hard disks, mechanics and materials problems will be discussed that are encountered during flying of a magnetic recording head at a head disk separation on the order of 1 nano meter. In order to increase the storage density further, the flying height of the read/write element must be reduced to less than 1 nm, and the track width to less than 20 nm (500,000 tracks per inch). To achieve sub-nano meter head disk spacing, the flying height of the head disk interface is controlled using the so-called thermal flying height control technology. In this approach, a controlled thermal deformation of the slider is achieved in the read write area of the slider by energizing a miniaturized resistance heater, causing a reduction in the flying height of the read write element to the order of 1 nm. Voltage biasing will be descussed to minimize materials transfer at the head disk interface. Another approach to achieve higher storage densities is the use of heat assisted magnetic recording where the magnetic medium is heated up to the Curie temperature just prior to recording using a laser beam. Current and future problems in the mechanics and materials area of information storage on hard disks will be presented.

2:40pm **E1-2-ThA-5 Frictional Anisotropy of MoS_2 During Sliding: A Molecular Dynamics Study on the Atomistic Understanding of Frictional Mechanisms***, **Victor Claerbout**, P Nicolini,* Czech Technical University in Prague, Czech Republic

The tribological characteristics of molybdenum disulfide (MoS_2) as solid lubricants are well-described starting from the discovery of the super low friction behavior of MoS_2 by Martin et al. in 1993 [1]. However, despite numerous experimental and theoretical efforts, a fundamental understanding of the frictional mechanisms at the nanoscale is lacking.

In this contribution, we aim to elucidate the phenomena taking place at the nanoscale when several layers of MoS_2 slide atop another. In particular, by means of molecular dynamics simulations, we studied the effect of rotational sliding anisotropy [2] (i.e., the changing frictional behavior upon introducing a misfit angle between the layers or by varying the relative sliding angle) on the energy dissipation due to friction. We simulated different sliding conditions (varying e.g. normal load) in order to highlight their effect on the lubricating properties. These results will help on the one hand to identify the fundamental mechanisms that govern friction at an atomistic level, as well as providing guidelines for the design of novel layered materials with improved tribological properties.

[1] J.M. Martin et al., Phys. Rev. B, 48, 10583(R) (1993). [2] Onodera et al., J. Phys. Chem. B, 114, 15832 (2010).

3:00pm **E1-2-ThA-6 Effect of the Presence of Small Molecules on the Entangled Electronic and Dynamic Features in Layered MX_2 Transition Metal Dichalcogenides: Systematic Quantum Mechanic Ab Initio Smulations***, **Jamil Missaoui**, A Cammarata,* Czech Technical University in Prague, Czech Republic

Great attention has been paid to the problem of friction in materials because of its enormous practical and technological importance in a vast range of scales including nanomaterials. In particular, control of intrinsic friction is mandatory in nano-electro mechanical devices (NEMS), mainly based on multi-layered Transition Metal Dichalcogenides (TMD). In this perspective, the present work is aimed to study the entangled electronic and dynamic features of selected TMD in the presence of small molecules of contaminants from the atmosphere.

We conducted systematic quantum mechanic ab initio simulations on prototypical layered MX2 (M = transition metal, X = chalcogen anion) TMDs with hexagonal structure in the presence of small molecules in the inter-layer region. We combined group theoretical analysis and phonon band structure calculations with the characterization of the electronic features using non-standard methods such us orbital polarization and the recently formulated bond covalency and cophonicity analyses. We will then study how the vibrational frequencies of the pristine material are shifted in the presence of the contaminant, by relating such shift to the nanoscale friction between adjacent MX2 layers. Finally, we will present guidelines on how to engineer intrinsic friction in TMDs at the atomic level.

Thanks to the generality of the used simulation protocol, the outcomes of the present study can be exploited to harness the macroscopic response of electro-dynamic entangled systems; the latter find application in fields beyond tribology based on physical phenomena like metal-insulator transition, second harmonic generation, and exciton effects (optoelectronics), among others.

3:20pm **E1-2-ThA-7 Nanoscale Frictional Properties of Ordered and Disordered MoS_2***, E Serpini, A Rota,* Università di Modena e Reggio Emilia, Italy*; S Valeri,* Istituto CNR-NANO S3, Italy*; E Ukraintsev,* Academy of Science of the Czech Republic, Czech Republic*; B Rezek,* Czech Technical University in Prague, Czech Republic*; T Polcar,* University of Southampton, UK*; **Paolo Nicolini**,* Czech Technical University in Prague, Czech Republic

One third of energy produced by industrial countries is lost as friction. High wear caused by friction means approx. 35% of industrial production is used to replace degraded products, whilst causing the breakdown of machinery, resulting in safety risks and environmental pollution. Controlling and reducing friction is a fundamental step in attaining the sustainable development of our society, as detailed in the Brundtland report. In this contribution I will present the results of a study on the nanometric sliding of molybdenum disulfide against itself both from the experimental and from the computational point of view. The differences between ordered material (single crystal) and disordered material (sputtered coating) were investigated. Tribological experiments were performed using Lateral Force Microscopy. Atomic Force Microscopy tips modified by sputter deposition of molybdenum disulfide were used for the first time. This feature opened up the possibility for close comparison with classical molecular dynamics simulations. In both cases, the coefficient of friction for the ordered system in inert conditions was found to be smaller than for disordered system. This result demonstrates the impact of morphology at the nanoscale and highlights the importance of molecular dynamics as a diagnostic and predictive tool in nano-friction. Furthermore, experiments show that the effects of the environment on nanoscale friction are reduced with respect to the macroscale case. These findings can expedite the process of fabricating molybdenum disulfide-based coatings with superior tribological properties, with the ultimate aim of reducing the energy dissipation due to friction.

3:40pm **E1-2-ThA-8 Electrical Tuning of Vibrational Modes in Transition Metal Dichalcogenides*, Florian Belviso,*** Advanced Material Group, Czech Technical University in Prague, Czech Republic

Transition metal dichalcogenides (TMDs) have been shown to be a promising source of applications in multiple fields, such as nanoelectronics, photonics, sensing, energy storage, and opto-electronics.

We investigated the atomic scale tribological properties of TMDs, using ab-initio techniques. Such compounds are formed by triatomic layers with MX2 stoichiometry (M: transition metal cation, X: chalcogen anion) held together by van der Waals forces.

We considered 6 prototypical MX2 TMDs (M=Mo, W; X=S, Se, Te) with hexagonal P63/mmc symmetry, focusing on how specific phonon modes contribute to their intrinsic friction. Within the DFT framework, we described the exchange-correlation interaction energy by means of the PBE functional, including long range dispersion interactions in the Grimme formulation (DFT-D3 van der Waals).

We identified and disentangled the electro-structural features that determine the intra- and inter-layer motions affecting the intrinsic friction by means of electro-structural descriptors such as orbital polarization, bond covalency and cophonicity.[1]

We show how the phonon modes affecting the intrinsic friction can be adjusted by means of an external electrostatic field. In this way, the electric field turns out to be a knob to control the intrinsic friction.

We also show the structural distortion induced by some various cation substitution.

The presented outcomes are a step forward in the development of layer exfoliation and manipulation methods, which are fundamental for the production of TMD-based optoelectronical devices and nanoelectromechanical systems.

[1] Cammarata, Antonio and Polcar, Tomas (2015) DOI 10.1039/C5RA24837J

4:00pm **E1-2-ThA-9 On the In-situ Formation of Transition Metal Disulphides in Lubricated WN or WC Coating Contacts*, Bernhard Kohlhauser,*** TU Wien, Institute of Materials Science and Technology, Austria*; M Rodríguez Ripoll,* AC2T research GmbH, Austria*; H Riedl, C Koller, N Koutna,* TU Wien, Institute of Materials Science and Technology, Austria*; G Ramirez, A Erdemir,* Argonne National Laboratory, USA*; C Gachot,* TU Wien, Institute for Engineering Design and Logistics Engineering, Austria*; P Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria

In recent years, solid lubricants such as transition metal dichalcogenides have attracted attention in form of nanoparticle additives for conventional oil-based lubricants. Those nanoparticle additives entail several disadvantages, including the need to compose a stable dispersion. An in-situ formation of lubricating solid compounds via a tribochemical reaction path between a coating and conventional S containing extreme pressure additives could prove to be much more advantageous.

While MoS_2 can easily be formed on metallic Mo surfaces, the conditions in lubricated tungsten contacts are not severe enough to produce WS_2. A new generation of functional coatings is helping to overcome this energetic barrier, which is linked to the formation of intermediate tungsten oxide phases. WN and WC based coatings are able to facilitate this in-situ formation of WS_2 and combine excellent mechanical properties with an optimization of friction and wear via the formation of a low friction tribofilms.

The coatings were prepared by magnetron sputtering and their mechanical, structural and chemical properties were investigated with nanoindentation, energy dispersive x-ray spectroscopy, X-ray diffraction, and transmission electron microscopy.

The tribofilms, resulting from lubricated pin on disk tests, were studied in detail and consist of a fraction of amorphous WS_2 and C based oil derived debris, but also of nanocrystalline WS_2 domains along the surface. These lubricating WS_2 sheets lead to a low coefficient of friction around 0.05 and the tribofilm protects coating and counter body from any wear, even after 100 h of testing.

4:20pm **E1-2-ThA-10 Tribological Investigations of Coated Roller Finger Followers using Application Oriented Valve Train Test*, Ricardo H. Brugnara*,** *E Schulz, L Dobrenizki, N Bagcivan, C Geers,* Schaeffler AG, Germany

Due to the increasing demand to reduce emissions, friction reduction is an important topic in the automotive industry. Among the various possibilities to reduce mechanical friction, the usage of a low-viscosity lubricant in the engine is one option. Thus, continuously lower viscosity lubricants are being developed and offered on the market. Other approach is to adjust the properties of the components using surface technology in order to minimize friction losses and meet the more stringent environmental requirements. Coated components using thin film vacuum technology offers the possibility to reduce CO_2-emissions and fuel consumption of the vehicle by mandatory lightweight design, reducing friction losses in tribological contacts. In present study, uncoated and DLC (Diamond-like Carbon) coated roller finger followers were investigated for the first time using application oriented driven cylinder head tests with 0W20 low viscosity oil under relevant conditions. The results show a significant friction reduction in rolling contact with coated cam rollers compared to the uncoated refence.

4:40pm **E1-2-ThA-11 Physical Understanding to Nano-friction of C:H/D Thin Films: Coupling Mechanism by Atomic-scale Vibration Damping***, F Echeverrigaray, S de Mello,* Universidade de Caxias do Sul, Brazil*; F Alvarez,* Universidade Estadual de Campinas, Brazil*; A Michels,* ***Carlos Figueroa*,** Universidade de Caxias do Sul, Brazil

Friction phenomenon is a complex manifestation of the nature originated in energy dissipation events owing to the lost work of non-conservative forces. In spite of phenomenological laws describe the friction force at different scales, the fundamental physical understanding of such a phenomenon still did not achieve consensus. Phononic, electronic, magnetic and electrostatic effects were considered and theoretical models were developed in order to explain the nano-friction behavior of materials. The surface structure of deuterated and/or hydrogenated amorphous carbon (a-C:D/H) thin films in air, which plays an important role in nanoscale friction research, is constituted by deuterium and/or hydrogen terminated bonds and physisorbed oxygen, nitrogen and water molecules. There are well established models to explain the tribological behavior of carbon-based thin films in different atmospheres, however, the fundamental physical mechanism at the interfacial atomic-scale remains open. In this study, we report the friction forces at the nanoscale on amorphous carbon thin films with different [D]/[C] and [H]/[C] contents by nanoindentation followed of unidirectional sliding (NUS) and friction force microscopy (FFM). Two different experimental setups are reported. Firstly, for samples where hydrogen was replaced by deuterium in the thin film the friction force decreases with the increasing of deuterium content, this behavior is associated to a fononic phenomenon owing to isotope effect. Secondly, for samples where hydrogen content is increased at the surface, the friction force decreases with the increasing of the ratio H/C at the surface, which is explored by an electronic interaction analysis. We discuss these two different frictional damping mechanisms by dissipation effects associated with phonon/van der Waals (vdW) coupling by sliding interface polarizability.

Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room Grand Hall - Session EP-ThP

Tribology and Mechanical Behavior of Coatings and Engineered Surfaces (Symposium E) Poster Session

EP-ThP-2 Deposition of DLC/Si-N Composite Films Synthesized by Sputtering-PBII Hybrid System and Their Thermal Stability*, **Anas Melih**, K Yamada, S Watanabe,* Nippon Institute of Technology, Japan

Diamond-like carbon (DLC) is a metastable amorphous film that exhibits unique properties. However, many limitations exist regarding the use of DLC, for example, its tribological characteristics at high temperature, as well as its limited thermal stability. In this study, silicon/nitrogen incorporated diamond-like carbon (DLC/Si-N) composite films are studied, taking into account the thermal stability and tribological performance of these films compared with pure DLC. All the films were synthesized using RF magnetron sputtering combination with PBII techniques (so-called Sputtering-PBII Hybrid System). High purity of Silicon nitride (99.9%) disk was used as a target with RF power of 500-700 W. The substrates were also applied with negative-pulsed bias voltage of 5 kV. The mixtures of Ar-CH_4 were used as reactive gas by varying CH_4 partial pressure between 0 and 0.15 Pa, while total gas pressure and total gas flow were fixed at 0.30 Pa and 30 sccm, respectively. The structure of the films was characterized using Raman spectroscopy. The thermal stability of the films was measured using thermogravimetric and differential thermal analysis (TG-DTA). The friction coefficient of the films was assessed using ball-on-disk friction testing. The results indicate that DLC/Si-N composite films present better thermal stability due to the presence of Si-O networks in the films. The DLC/Si-N (about 11 at.%Si, 18.5 at.%N) film was showed good thermal stability in an air atmosphere with increasing temperature until 800°C. Further, the films exhibit excellent tribological performance at 500°C in an air atmosphere. It is concluded that the DLC/Si-N composite films improve upon the thermal stability and tribological performance of DLC at a high temperature .

EP-ThP-3 Mechanical and Tribological Performance of TiAlN, TaN and Nanolayered TiAlN/TaN Coatings Deposited by DC Magnetron Sputtering*, **Elbert Contreras**, J Cortínez, M Gómez,* Universidad de Antioquia, Colombia*; A Hurtado,* Centro de Investigación en Materiales Avanzados CIMAV, Mexico

Nanoscale multilayer systems have become the most important way to increase the mechanical and tribological performance of wear protective coatings. In the present research, nanoscale TiAlN/TaN multilayer coatings were deposited by DC magnetron sputtering, controlling the substrate rotation speed in order to obtain different periods and to evaluate their effect on mechanical and tribological properties; additionally, monolayer TiAlN and TaN coatings were deposited to compare the effect of multilayer architecture on the coatings performance. SEM images showed a well define columnar and homogenous microstructure, it was possible to observed the multilayer architecture with higer bilayer periods. TEM images exhibited well defined interface and diffusion between both TiAlN and TaN layers. A high crystalline coatings, change in the growth direction of coatings and residual stresses was the most relevant results obtained by XRD. Regarding to the residual stresses, it was observed that monolayer coatings exhibit high compressive stresses reaching values up to 8 GPa. On the other hand, the residual stresses of nanoscale multilayer coatings exhibit considerable lower values and decrease progressively as the bilayer period of the coatings decreases, reaching values below 2 GPa. TiAlN and TaN coatings exhibited hardness of 16 GPa and 17 GPa, respectively, while TiAlN/TaN coatings showed a progressive increase as the coating period decreases, reaching values up to 22 GPa with bilayer periods lower than 10 nm. Scratch test results showed that all nanoscale multilayer coatings exhibit better adherence compared to TiAlN and TaN monolayer coatings. Additionally, it was also observed a slight tendency to increase the adherence once the bilayer period decreases reaching values up to Lc = 42 N. Fracture toughness was evaluated by nanoindentation, it was possible to calculate a significant improvement in the toughness of multilayer coatings and a significant increase in the H^3/E^2 ratio. With respect to the tribological performance, it was possible to observe a decrease in friction coefficient and wear rates of nanoscale multilayer coatings compare to TiAlN and TaN monolayer coatings. Using cross-section FIB it was possible to observe initial deformation in the constituent layers followed by the propagation of cracks along the interfaces between TiAlN and TaN layers, in nanoindentation tests, scratch tests and tribological tracks.

EP-ThP-4 Development of Catalytically Active Nano-Composite Coating for Severe Boundary Lubricated Conditions of Hydraulic Fluids*, V DaSilva, **Osman Levent Eryilmaz**, A Erdemir,* Argonne National Laboratory, USA

Applying thin coatings onto bulk materials is a surface benefactor favorable in tribology because of its ability to lower friction and copiously improve wear performance. These phenomena result in more reliable mechanical systems and improve energy efficiency. In this work, Vanadium Nitride - Copper coatings were produced and optimized (power of each target was adjusted to achieve a range of Cu concentration within the hard nitride phase) using HIPIMS magnetron sputtering system. The thin coatings were deposited onto 52100 steel flat, cylinders, and ball samples for tribological testing. Characterization such as surface roughness, composition, coating thickness, and adhesion were analyzed using a wide range of characterization techniques prior to testing. The coatings were evaluated in hydraulic fluids under unidirectional sliding (ball on flat) using two different test configurations. The results showed that, use of coating on both static and moving surfaces significantly improved wear resistance and lowered the coefficient of friction when tested under severe conditions (1 GPa maximum Hertzian contact pressure). Post-test microscopy and profilometry analysis confirmed ultralow wear on sliding surfaces. Furthermore, the VN-Cu coated surfaces showed an astounding 30-40% reduction in coefficient of friction compared to baseline 52100 ball on 52100 flat in hydraulic fluid.

EP-ThP-5 Size-Independent High Strength of CuTi/Ti Metallic Glass/Crystalline Nanolayers*, M Abboud,* Middle East Technical University, Turkey*; A Motallebzadeh,* Koç University, Turkey*; **Sezer Özerinç**,* Middle East Technical University, Turkey

Thin film metallic glasses (MG) offer a wide design space for the development of hard, corrosion resistant and biocompatible coatings. However, one of the major disadvantages of MGs is their brittle nature. Utilizing a nanolayered MG – crystalline structure is a promising approach for improving the ductility of these materials. Hardness of these nanocomposites usually increases with decreasing layer thickness, and it is lower than that of the corresponding monolithic MG. In this work, we demonstrated a nanolayered model system composed of CuTi MG and nanocrystalline Ti layers (CuTi/Ti) that shows unusually high hardness, comparable to that of monolithic CuTi MG. Furthermore, we did not observe any significant dependence of strength on layer thickness.

We prepared thin films of nanocrystalline Ti, CuTi MG, and nanolayered CuTi/Ti. A magnetron sputterer deposited 1 µm-thick films on oxidized silicon substrates, and layer thickness was varied in the range 10–100 nm. X-ray diffraction and electron microscopy verified the microstructure with alternating layers, and nanoindentation experiments measured the mechanical properties.

Nanocrystalline Ti sample has an average grain size of ≈20 nm and the grain size of Ti layers in the CuTi/Ti samples varies in the range 5–16 nm; monotonically increasing with increasing layer thickness. Hardness of all CuTi/Ti nanolayers are in the range 7.1–7.3 ±0.3 GPa with no observable layer thickness dependence; and are comparable to that of monolithic CuTi MG (7.0 ±0.3 GPa). On the other hand, 1 µm-thick nanocrystalline Ti has a hardness of only 0.9 GPa. An order of magnitude higher hardness of the nanocomposite when compared to the crystalline Ti suggests that the confinement of hexagonal close-packed Ti in between amorphous layers results in unexpected levels of extrinsic strengthening. In order to have a comparison, we also prepared nanolayered CuTi MG/crystalline Cu samples. These layers are softer than CuTi for all layer thicknesses, and show the usual size dependence of increasing hardness with decreasing layer thickness, in the range 5.1–6.3 GPa. These differences between the samples containing HCP Ti layers and FCC Cu layers suggest that crystal structure plays an important role in the mechanical behavior of nanolayered MG-crystalline composites.

The results demonstrate that by the appropriate selection of the constituent layers, it is possible to design size-independent high strength nanolayered metals. This enables the opportunity of engineering the layer thicknesses for optimizing other properties of nanolayers such as ductility, corrosion resistance and biocompatibility for application requirements.

EP-ThP-6 Extended Crack-free Tensile Deformation of Ultrathin Metallic Glass Films Due to an Intrinsic Size Effect*, **Oleksandr Glushko,*** Erich Schmid Institute of Materials Science, Austria*; M Mühlbacher,* Montanuniversität Leoben, Austria*; C Gammer, M Cordill,* Erich Schmid Institute of Materials Science, Austria*; C Mitterer,* Montanuniversität Leoben, Austria*; J Eckert,* Erich Schmid Institute of Materials Science, Austria

Although metallic glasses (MGs) exhibit a unique combination of mechanical and chemical properties (high strength, hardness, elastic strain, wear and corrosion resistance, biocompatibility), their application as structural or functional materials is hindered by the lack of ductility which leads to catastrophic brittle-like fracture. When the size of a MG sample is reduced below some critical value, typically of the order of a few hundred nanometers, then considerable ductility can be observed. However, this size effect was demonstrated so far mostly by nanomechanical testing inside a transmission electron microscope using samples prepared by focused ion beam (FIB) milling. Whether the ductile-like behavior of submicrometer-sized metallic glasses is a real "intrinsic" size effect or it is rather caused by extrinsic factors like sample shape, ion beam effect or parameters of the testing setup is currently a subject of extensive discussions in the community.

In this contribution the tensile properties of thin film PdSi MGs grown by sputter deposition on a polymer substrate are considered. The integrity of the MG films during stretching was monitored by in-situ measurements of the electrical resistance. Although the 250 nm thick films fail in a brittle manner at 2% strain, considerable local ductility originating from the substrate constraint is observed. A strong size effect on the deformation behavior appears when the film thickness drops below 16 nm. The 7 nm thick films with the same composition show a crack-free deformation up to a strain of 7%. Even at higher strains no brittle-like failure but rather short and isolated cracks are observed. Cyclic tensile loading revealed extreme fracture resistance of ultrathin amorphous films showing no cracks after 30000 stretching cycles with a strain amplitude of 2%. Since all tests are performed at ambient conditions on films deposited using an industrially scalable process, the demonstrated size effect can be directly utilized for applications, such as protective coatings, nanoelectromechanical devices or half-transparent conductive layers for flexible electronics.

EP-ThP-11 Effect of Surface Treatments on AISI H13 Steels*, **Marco Antonio Doñu Ruiz,*** Universidad Politecnica del Valle de México, Mexico, México*; M Buenrostro Arvizu,* Universidad Autonoma Metropolitana Azcapotzalco, Mexico*; N Lopez Perrusquia,* Universidad Politecnica del Valle de México, Mexico, México*; V Cortés Suárez,* Universidad Autonoma Metropolitana Azcapotzalco, Mexico*; C Torres San Miguel,* Instituto Politecnico Nacional, Mexico*; G Pérez Mendoza,* Universidad Politecnica del Valle de Mexico

Mechanical properties can be improved by thermochemical treatments, the present work studied the effect of surface treatment on AISI H13. Nitriding was performed according to TENIFER® process under two conditions; i) samples of were employed in the salt bath component at temperature of 853 K with exposure time of 1h 3min ii) sample were austenized in a vacuum furnace at a temperature of 1283 K for 90 minutes and cooled with nitrogen to 333 K. After all the samples were tempered, the first was carried out at 813 K and the second at 878 K, with 2 h, respectively. After hardening and tempering (HT) , the samples HT were nitride (HTN).

Boro nitride coating was applied on samples on AISI H13 in two stage: i) samples were boride by paste dehydrated pack at temperatures 1173 K for 3 hours and then nitriding on sample boride at temperature of 853 K with exposure time of 1h 30 min.

The microstructural and phases composition were characterized using scanning electron microscopy (SEM) and X-ray diffractometer (XRD). The samples were mechanical characterization by three-point bend test and microhadness test.

Nitrided coating thicknesses are over thicknesses of 4.97 um with zone of diffusion of 52.8 um of thickness, for the case of boronitride a depth of 26.42 um is observed. For the condition AISI H13 hardening, tempering and nitriding a maximum bending stress of 10990 MPa was obtained in comparison with the AISI H13 as received with a value of 3677 MPa.

EP-ThP-12 Mechanical Properties and Fretting Corrosion of Zr/ZrN/CNx Hierarchical Multilayers Deposited by HIPIMS on Ti Biomedical Alloy*, **Martin Flores**, J Perez, O Jiménez, L Flores,* Universidad de Guadalajara, Mexico

The hierarchical multilayers of hard ceramic coatings can improve the adhesion to substrates and the tribocorrosion resistance of biomedical alloy as Ti6Al4V. The coatings deposited by HIPIMS have a more compact growth respect to films deposited by DC magnetron sputtering; this diminish the presence of pinholes and defects that permit to predict a reduction in permeability. The design of the multilayer was made with a top layer of CNx in order to reduce the friction coefficient. In this work we study the mechanical and fretting corrosion behaviour of Ti6Al4V biomedical alloys coated with multilayers of Zr/ZrN/CNx and Zr/ZrN deposited by HIPIMS (High Power Impulse Magnetron Sputtering). The fretting corrosion tests were made in fetal bovine serum (FBS) to simulate the proteins in synovial liquid. The tribocorrosion was studied using open circuit potential (OCP) and potentiostatic polarization in the passive region during the relative movement of samples. The friction coefficient was measured as a function of the applied potential. The worn surface at wear track was analysed by SEM, XRD and Raman spectroscopy. We report the results on composition and structure of tribolayer and removed material of the wear tracks, and the comparative study in mechanical properties fretting corrosion and friction behaviour of coatings of Zr/ZrN and Zr/ZrN with a top layer of CNx.

EP-ThP-13 Quantum Tools for Life-Time Prediction of Coatings and Thin Films*, **Norbert Schwarzer,*** SIO, Germany

Everybody who ever tried to do some life-time prediction on parts subjected to erosion or tribology or any other form of complex and potentially multi-body interaction full well understands and values Mark Twain's famous dictum about the simple fact that making predictions is very complicated… especially if they concern the future. The smaller the objects and the more complex their internal structure the even more complicated this task becomes. In thin-film physics the most principle uncertainties come on top of the already rather nonlinear and often chaotic behavior the objects of interest are subjected to.

Instead of seeing this increase of complexity due to the incorporation of roughness, defects, impurity and quantum effects as an additional problem in our efforts to come to better life-time predictions with respect to all sorts of coating-applications, this author actually saw an interesting potential in the apparently tedious "add-on-effects" coming into play with smaller and smaller scales.

By incorporating quantum theoretical concepts into highly sophisticated physical models [1] we obtained a very compact, rather general and powerful tool to handle practical applications in many different fields, leading to a much more holistic uncertainty budget calculation and – as a surprise – even a more comfortable and secure life-time prediction.

[1] N. Schwarzer, "The Theory of Everything - Quantum and Relativity is everywhere – A Fermat Universe", Pan Stanford Publishing, July 2018, ISBN-10: 9814774472

EP-ThP-16 Structure and Fretting Wear Behavior of CuNiIn/MoS_2-Ti Multilayers Fabricated by Magnetron Sputtering Method*, **Chunbei Wei**, Q Li, S Lin, H Hou, M Dai,* Guangdong Institute of New Materials, China

Fretting denotes a tribological phenomenon related to movements of small amplitudes between two surfaces in contact. This working condition occurs in many mechanical assemblies where the parts are occasionally subjected to a vibrating environment or are sustaining variable stresses directly. It often results in damage that may lead to premature component failure. A thick soft CuNiIn coating prepared by plasma sprayed is usually used to cover engine components from fretting due to its great capacity of accommodation by plastic deformation. However, CuNiIn coating has limited life because of its high friction coefficient. Some researches combine CuniIn+polymer bonded lubricant MoS_2 to improve the tribological behavior due to the cohesion, ductility and adhesion of third bodies inside the contact.

In this paper, CuNiIn/MoS_2-Ti multilayer was fabricated by magnetron sputtering method. As a comparison, CuNiIn monolayer and MoS_2-Ti monolayer was also prepared. The linear fretting wear was used to study the fretting wear behavior of the coatings. The results show that the interface of multilayer prevented the growth of thick columnar crystal of CuNiIn interlayer and MoS_2-Ti interlayer, whereas the monolayer showed thick columnar structure. A compact, fine crystal structure has formed for CuNiIn/MoS_2-Ti multilayers. The microhardness of the multilayers was in the range of 350~500HV, which was higher compared with that of the CuNiIn and MoS_2-Ti monolayer. After 12000 cycles of fretting wear, the friction coefficient of CuNiIn monolayer was more than 1.0, and its wear trace depth reached to 108μm, indicated the failure of the coating. However, the friction coefficient of MoS_2-Ti monolayer was about 0.1, and the wear trace depth was 4.5μm. MoS_2-Ti monolayer exhibited good lubricant properties, leading to the improvement of the tribological performance. The friction coefficient of CuNiIn/MoS_2-Ti multilayer was lower to 0.07, and the wear trace depth was 0.5 μm, demonstrated that the better wear properties of the multilayer compared with that of the monolayer. These can attribute to the more compact structure and higher ductile of the multilayers, as well as its good lubricant characteristic.

EP-ThP-17 Contact-focusing Electron Flow (CFEF) Induced Near-zero Running-in for Low Friction of Carbon-steel contact Interface*, **Dongfeng Diao,*** Institute of Nanosurface Science and Engineering, Shenzhen University, China

Under air condition, a-C film sliding against steel surface often shows high friction coefficients (μ=0.1~0.3), which largely impedes its potential in industrially. In this study, we report a new method of contact-focusing electron flow (CFEF) by applying direct current (DC) at the sliding interface between a-C film and steel ball to trigger the in-situ formation of nanosized graphene sheets, and induce a fast low-friction behavior. The developments of the friction behavior with different DC values and normal loads were examined. The typical friction coefficient dropped one order of magnitude from 0.2 to 0.02 and the run-in period was close to zero under CFEF-condition. The low friction interface, especially the carbon-transfer film was examine at nanoscale by using the newest detecting avenues. The nanostructure of the transfer films was observed by Cs-corrected TEM and EELS analysis. The elemental composition of the transfer film was investigated by using EDS, XPS and Raman spectra analysis. Based on these analyses, we found three key factors for the fast low friction (near-zero running-in). (1) CFEF excited the carbon structural transition from amorphous to graphene sheet at the contact area. (2) Friction transferred the nanosized graphene sheets to the steel ball surface. (3) CFEF-friction coupling effect supplied the nanosized graphene sheets into the sliding interface. This work shed light on the CFEF-method for the in-situ fabrication of nanosized graphene sheets at the carbon-steel contact interface for low friction with near-zero running-in period.

EP-ThP-18 Misinterpreting Size-effects during Coating Nanoindentation*, **Esteban Broitman,*** SKF Research & Technology Development Center, Netherlands

The hardness of a material is a multifunctional physical property depending on a large number of internal and external factors. The transition from macroscale to microscale, and from microscale to nanoscale indentation hardness measurement is accompanied by a decreasing influence of some of these factors and by an increasing contribution from others.

The Vickers indenter used in macro-indentation tests has been designed to give geometrically similar indentations (i.e. the strain generated within the material is independent of the load), so the hardness should be independent of the indentation size. This fact results to be true for macroscale indentations. However, for microscale indentations (loads of less than 1N), it is well established that the hardness decreases or, more frequently, increases with the decrease of the applied load. This effect is known as the *"indentation size effect"* (ISE). The same phenomena has also been observed during coating nanoindentations at very low loads (low indentation depths), using either Berkovich or cube-corner indenters.

The gradient plasticity theory attributes ISE to the evolution of the so-called geometrically necessary dislocations beneath the indenter, which gives rise to strain gradients that affect the measurements at low penetration depths. In this presentation we will show that most of the ISE reported in the literature are, in fact, related to artifacts originated from a wrong surface preparation that generates work hardening, or the lack of surface microstructural characterization, which leads to ignore the presence of surface roughness, grain precipitates, or very thin surface oxide layers. Furthermore, we will show also that ignoring pile-ups or the use of an incorrect indenter geometric calibration generate false ISE results. We conclude that most of reported ISE have been misinterpreted and can be suppressed when proper data interpretation and processing are used.

EP-ThP-19 e-Poster Presentation: Think You Have Produced DLC? Think Again!*, **Arman Mohammad Khan,** H Wu, Y Chung, Q Wang,* Northwestern University, USA

Carbon-containing tribofilms have been widely reported to form in lubricated tribological contacts. These films show the same Raman *D* and *G* signatures as those of graphite- or diamond-like carbon (DLC) films. As a result, these films are commonly assumed to be DLC. Our work has revealed that this interpretation may not be always correct. In our experiments, we formed such tribofilms in standard pin-on-disk tribotesting using steel counter-faces and polyalphaolefin (PAO) base oil with cyclopropanecarboxylic acid (CPCa) as an additive. Raman spectra obtained from these tribofilms have *D* and *G* features identical to those from DLC. Multiple analytical techniques (micro-FTIR, mass spectrometry, and proton NMR) coupled with reactive molecular dynamics simulations demonstrate that these tribofilms are not DLC, but are in fact high molecular weight hydrocarbons acting as a solid lubricant.

EP-ThP-20 Mechanical and Tribological Properties of Cr-Al-Si-N-O Coatings Prepared by Arc Ion Plating for Cutting Tools*, **Jun-Ho Kim,** W Kim,* Korea Institute of Industrial Technology (KITECH), Republic of Korea

Quinary Cr-Al-Si-N-O nanocomposite films were deposited onto WC-Co substrate by a filtered arc ion plating system using $CrAl_2$ and Cr_4Si composite targets under N_2/Ar atmosphere. XRD and XPS analyses revealed that the synthesized Cr-Al-Si-N-O films were nanocomposite consisting of nanosized (Cr,Al,Si)N crystallites embedded in an amorphous Si_3N_4/SiO_2 matrix. The hardness of the Cr-Al-Si-N-O films exhibited the maximum hardness values of ~40 GPa at a Si content of ~2.78 at.% due to the microstructural change to a nanocomposite as well as the solid-solution hardening. Besides, Cr-Al-Si-N-O film with Si content of around 2.78 at.% also showed perfect adhesive strength value of 109 N. These excellent mechanical properties of Cr-Al-Si-N-O films could be help to improve the performance of machining tools and cutting tools with application of the film. Also X-ray diffractometer (XRD) analysis was conducted to investigate the crystallinity and phase transformation of the films. Moreover, it was found that the improved nanohardness and the H/E ratio contributed to excellent wear resistance of the coatings. The friction coefficient and wear rate of the Cr-Al-Si-N-O coatings first decreased and then increased with increasing silicon content. The friction coefficient and wear rate were also mainly related to the lubricant wear debris in this work.

EP-ThP-22 Friction Property of Si-DLC with Scratch Damage Before and After Local Repairing Deposition to the Scratch Scar*, H Takamatsu, K Tanaka,* ***Akihiko Ito,*** *H Kousaka, T Furuki,* Gifu University, Japan

Diamond-Like Carbon (DLC) has excellent mechanical properties such as high hardness (over 10GPa), high wear resistance, and low friction. However, DLC film has low impact resistance and toughness because of its high hardness and brittleness, and thus it is often damaged by cracking from film surface and peeling from base material.

DLC film with local damages is repaired through the following process: (1) Removal of all the DLC film, (2) Recoating of new DLC film. However, this process is not efficient. We have proposed a new way of repairing, or recoating only to local damaged points of DLC by using a micro coating device. In this paper, we discuss the friction property of Si-DLC on which a local damaged point is repaired by recoating.

A local damage was introduced to Si-DLC pre-coated steel disk (SUJ2, JIS) by scratching at an almost constant load. Recoating of Si-DLC was conducted to the Si-DLC disk with a slit mask so that only the area near the scratch is recoated.

In order to evaluate the friction behavior of pre-coated, damaged and repaired Si-DLC films, these films were slid against a steel ball (SUJ2, JIS) at a vertical load of 15N and a rotation speed of 10m/min by ball on disk friction tester.

During running-in process, damaged Si-DLC showed frequent fluctuation of friction coefficient, which appeared from the sliding distance of about 60m. After the process has done, large increase of friction coefficient was sometimes confirmed with passing through the scratch scar. On the other hand, such fluctuation and unstable transition of friction coefficient were not confirmed in the repaired Si-DLC.

Transfer film formed onto the mating steel ball surface is considered to easily re-adhere to the metal exposed part in the damaged Si-DLC. Such transfer film detached from the ball surface can easily stick back to the ball surface, because of initial oxide film on the ball which prevents the formation of transfer film is already removed during the initial stage of sliding. We assume the fluctuation of friction coefficient in the damaged Si-

DLC was caused by such detachment and re-attachment of transfer film at the sliding interface. In addition, we consider that such detachment of transfer film was suppressed in the repaired Si-DLC because the metal exposed part is covered by recoating of Si-DLC. As result, it is possible that partially repairing local damaged DLC shows better friction properties.

EP-ThP-23 Raman Scattering Characterizes Thermally Annealed HiPIMS Sputtered MoS2 Coatings*, **Henning Moldenhauer**, W Tillmann, A Wittig, D Kokalj, D Stangier, A Brümmer, J Debus,* TU Dortmund University, Germany

Omnipresent friction forces and wear limit the service time of machine parts. The usage of lubricants increases the service time remarkably due to a reduction in the wear. In that context, solid lubricants, like MoS_2 coatings grown by physical vapor deposition (PVD), are highly promising. However, the friction coefficient and, consequently, the lifetime of the coating depend on its oxidation resistance which in turn depends on several microscopic parameters, like its structure. In order to produce highly oxidation resistant coatings, high-power impulse magnetron sputtering (HiPIMS) is used. Their structural properties at the nanoscale are characterized by laser-light scattering methods; in particular, Raman scattering studies on HiPIMS sputtered MoS_2 thin films are performed aiming at their structural and tribological properties under multiple annealing conditions.

Raman scattering spectroscopy is a non-destructive and contactless tool for identifying the structure, morphology and chemistry of material surfaces. The material's quantized lattice vibrations are laser-excited and optically measured, thus generating a physicochemical fingerprint of the surface at the atomic scale. Raman scattering spectroscopy provides a high spatial resolution of about one micrometer and can be used for practically any sample geometry.

Using this technique, a microscopic layering of MoS_2 is detected: Interlayer-phonon modes at low frequency (38 cm^{-1}) build up for increasing annealing temperatures of the coatings (until 600°C). Changes in the intensity ratio of the in-plane and out-of-plane Raman modes moreover hint at crystal symmetry changes. To assess the tribological performance, ball-on-disc experiments are performed in combination with Raman scattering. A dependence of the friction coefficient on the annealing temperature and the layering of the MoS_2 is found. Furthermore, the MoS_2 typical needle-like structure and a denser morphology of the MoS_2 thin films compared to a DC sputtered reference are revealed by scanning-electron microscopy. A hexagonal crystallization structure and the crystallite size are evaluated from X-ray diffraction.

EP-ThP-24 Friction Reduction in Sliding Between Si-DLC vs. Steel Ball by Ar Plasma Irradiation Using Microwave-excited Atmospheric Pressure Plasma Jet*, T Hibino, **Hiroyuki Kousaka**, T Furuki,* Gifu University, Japan*; J Kim, H Sakakita,* National Institute of Advanced Industrial Science and Technology (AIST), Japan

Diamond-like carbon (DLC) has widespread applications in many fields due to its excellent mechanical properties such as high hardness, low friction, chemical inertness, and so on. Recently, DLC is applied to machine parts as surface coating to improve frictional property. The interface between DLC and mating surface shows low friction through running-in period, in which shear strength at the interface decreases gradually; in other words, the interface between as-deposit DLC and mating surface does not show low-friction from the very beginning of sliding. Since high-friction during running-in period may cause severe damage to sliding interface such as the fracture of DLC coating, shortening of running-in period is desired. In our previous work, Okumura et al. investigated the influence of atmospheric He plasma irradiation to the sliding interface between a polyacetal ball and Si-doped DLC disk, demonstrating that the running-in period is shortened by plasma irradiation [1]. In this work, we further tried to use plasma irradiation for shortening the running-in period in the sliding between a steel ball and Si-doped DLC disk. A Si-doped DLC (a-C:H:Si) with a Si content of 27 at % was coated by using DC plasma enhanced chemical vapor deposition (PECVD) onto a steel disk (SUS304, JIS) 25 mm in diameter. The Si-DLC disk was slid against a stainless-steel ball (SUS440C, JIS) 8mm in diameter under dry condition at a normal load of 1 N and rotation speed of 0.67 m/s for 1800 m. During the initial sliding distance of 100 m, atmospheric Ar plasma was irradiated to the sliding track on the Si-DLC disk by using microwave-excited atmospheric pressure plasma jet [2]. In the case of plasma irradiation, friction coefficient decreased to 0.1 rapidly just after stopping the plasma irradiation and it was kept from 100 to 1800 m, or the end of sliding test; on the other hand, friction coefficient without plasma irradiation was always higher than 0.1 and fluctuated more largely from 100 m to 1800 m. It was shown in the sliding between a steel ball and Si-doped DLC disk that the plasma irradiation shortened the running-in period and decreased friction coefficient. (The authors gratefully acknowledge the funding by JST CREST, Japan.)

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[2]. J. Kim, et. al, Microwave-excited atmospheric pressure plasma jet with wide aperture for the synthesis of carbon nanomaterials, Japanese Journal of Applied Physics 54, 01AA02 (2015).

EP-ThP-27 Taguchi Method to Study Effects of Plasma Surface Texturing on Friction Reduction of Cast Iron at High Speed Sliding Lubricated Conditions*, W Zha, C Zhao, R Cai, **Xueyuan Nie**,* University of Windsor, Canada

Cathodic plasma electrolysis (CPE) is used to create surface texture on cast iron for the purpose of friction reduction. Micro craters formed by the explosion of gas bubbles can generate hydrodynamic force that separate two sliding surface, increase the oil film thickness and thus, decrease the friction. The Taguchi method is used to find the optimal process parameters (voltage and roughness) for surface texturing. The orthogonal array and the signal-to-noise ratio are employed to study the effect of each process parameter on friction. The results show that with higher voltage and lower roughness, the friction coefficient can be reduced to a lower value.

EP-ThP-30 Test Rig Development For Static Friction Assessment At High Temperature*, M Azzi,* Lebanese University (UL), Lebanon*; E Bitar-Nehme,* Tricomat, Canada*; J Schmitt, T Schmitt, L Martinu, **Jolanta-Ewa Klemberg-Sapieha**,* École Polytechnique de Montréal, Canada

The oil and gas industry uses steam-turbine power generation valves are vital equipment components that are used to control the flow of steam. Sealing surfaces in the valve must withstand high contact and friction stresses at high temperature. The main cause of valve failure is the degradation of sealing surfaces that can result in valves not cycling on demand due to high static friction. Development of materials or coatings with high tribological performance (high wear resistance and low friction) at high temperatures is the key for manufacturing valves with long service life.

In the present work, a novel experimental test rig has been developed to rigorously investigate the evolution of static friction in a tribological contact at high temperature in terms of holding time and contact stress. Pin-on-Flat configuration has been adopted in the design with the flat sample being mounted in a furnace that heats up to 800ºC. The furnace moves vertically on a well-guided structure to bring the sample into contact with its counterface that moves in a linear motion generating friction.

Here, we present an approach to assess static friction, and we illustrate it by the results for stainless steel 304 and for Alumina counterface. The measurements showed that static friction increases with the number of passes to reach a plateau at 0.7 after a certain number of passes that depends on the contact stress. In addition, friction was shown to strongly depend on temperature and more importantly on the holding time at high temperature which might be related to processes such as diffusion that take place at the interface.

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 ^oC 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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