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

Friction, Wear, Lubrication Effects, and Modeling

Moderators: Albano Cavaleiro, University of Coimbra, Carsten Gachot, Vienna University of Technology, Giovanni Ramirez, Argonne National Laboratory, USA

8:00am **E1-1-1 Stress and Friction Modelling for Improved Nano-scratch Testing of Hard Coatings***, **Ben Beake,*** Micro Materials Ltd, UK*; V Vishnyakov,* University of Huddersfield, UK*; T Liskiewicz,* University of Leeds, UK

Nano- and micro-scale scratch tests have significant benefits over the more traditional macro-scale tests with 200 micron end radius diamond indenters. By employing smaller loads and sharper probes it is possible to greatly increase the sensitivity of the test to coating properties. Nevertheless, interpretation of the results can be complex without further analysis. In this paper we present (i) analytical modelling to assess the main stresses acting at the coating-substrate interface (von Mises, tensile and shear stresses) (ii) simulation of load-dependent friction. The modelling has been applied to different coating systems such as DLC on hardened steels and hard nanocomposite TiSiN on silicon. The stress modelling has been able to explain dramatic experimental differences in failure mechanisms with coating mechanical properties due to differences in tensile stresses at the interface and whether plastic flow initiates in coating or substrate. It has been possible to deconvolute the interfacial component of friction from the ploughing contribution and to accurate simulate the total frictional force by additionally considering the load-dependent transfer of load support to the front half of the probe as the deformation becomes less elastic in nature.

8:20am **E1-1-2 Wear Resistance and Solid Lubricity of Nanolayered Molybdenum Containing Nitride Coatings Deposited using Cathodic Arc Technique***, **Qi Yang,*** National Research Council of Canada, Canada

Molybdenum containing MoTiN, MoCrN, MoZrN and MoAlTiN nanolyered coatings, were deposited on the 17-4 PH stainless steel substrate by using cathodic arc evaporation technique. Pin-on-disc dry sliding tests were performed to investigate the coatings' wear resistance and solid lubricity. All these coatings, particularly MoTiN and MoAlTiN coatings, demonstrated wear resistance superior to and coefficient of friction significantly lower than the corresponding Mo-free TiN, CrN, ZrN and AlTiN coatings. For example, the specific wear rate of the MoAlTiN coating is less than 0.15% of that of AlTiN while its coefficient of friction is only 0.28 when compared to 0.60 of the AlTiN coating. The excellent tribological performance is contributed to the formation of the surface MoO_3 layer on the wear track due to the tribo-oxidation process. Further wear tests of the MoTiN and MoAlTiN coatings against Al_2O_3 ball revealed less improvement in wear resistance and less reduction in coefficient of friction. When tested against Si_3N_4 ball, both coatings, though showing noticeably better wear resistance than their corresponding Mo-free coatings, did not demonstrate low coefficient of friction. The scanning electron microscopy (SEM) and the energy dispersive X-ray spectroscopy (EDS) analyses of the wear track surfaces illustrated the importance of retaining a stable MoO_3 surface layer in order to maintain the beneficial effect of Mo on the tribological performance of the coatings.

8:40am **E1-1-3 Exploring Tribological Interactions – from Molecules to Engineering Applications***, **Daniele Dini,*** Imperial College London, UK **INVITED**

Tribological phenomena are governed by events and mechanisms which find their roots at the small scales, even more so in environments where mechanical and chemical effects are intimately coupled. For example, nano-scale thermal and particle emission events control the formation of antiwear additive films and oxidation; surface damage, such us crack initiation and wear, results from the accumulation of strain at dislocations level; corrosion events are triggered and controlled by molecular interactions. The key challenge addressed in this talk is the need for the development of robust methodologies for the integration of the skills and techniques recently developed by our modelling team at different scales (see e.g. [1-7]) to capture physical, chemical and mechanical processes and interactions across the scales via a multi-physics modelling strategy. Example of modelling methodologies developed and employed to solve problems at specific length- and time-scales will be presented before concentrating on coupling strategies to be adopted to shed light on macro-scale tribological events while zooming-in to understand their governing mechanisms.

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9:20am **E1-1-5 Mechanical Stability under Sliding Contact of Thin Multilayer with Weak Adhesion***, **Aymar Quarré de Boiry,*** Joint unit CNRS/Saint-Gobain UMR 125 - Surface of Glass and Interfaces, France*; D Dalmas,* École Centrale de Lyon – Laboratoire de Tribologie et Dynamique des Système, France*; J Faou, J Teisseire,* Saint-Gobain Recherche, France

To modify the surface properties of the flat glass (optical, thermal, electrochemical...), thin film deposition by magnetron sputtering is a technique increasingly widespread. For example, low emissivity glasses which are produced by Glass industry for many years allow reducing energy losses by blocking infra-red. An essential part of those functionalized glasses is a thin silver layer (ten nanometers) deposed by cathodic pulverization. However, these coatings have often low mechanical resistance toward contact loading (scratch) which can happen during manipulation or washing. Scratches are due to contact loading (friction) and are influenced by mechanical properties of the stack (modulus, toughness, adhesion …) [1]. However, a quantitative analysis of the damages is tough because of the complexity and the thinness of the layers (few nanometers). The idea developed during this study is to extend the understanding of the scratch phenomenon in order to improve the scratch resistance of thin multilayers by a method of interfacial patterning. Indeed, it has been recently showed that an alternation of weak adhesion areas (with silver) and strong adhesion areas (without silver) allows improving adhesion [2, 3].

In this study, the objective is to perform ball on plan tests to analyze and understand scratch mechanisms on multilayers thin film with low adhesion deposited on glass. Indeed, the glass transparency allows a direct visualization of scratching process during the tests. First, we focused on homogenous samples with a weak interface and we shows that the scratch is strongly influenced by the presences of brittle layers in the stack. Then, a photolithography protocol is used to pattern a ten nanometers silver layer inside a multilayer stack. In order to understand the scratch phenomenon and the contact between the ball and the layers, many parameters have been measured and their influences and evolution will be discussed: distance between the surface and the sphere, generation of debris, initiation morphology or width of the scratch.

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10:00am **E1-1-7 Tribochemical Investigation of Hydrogenated DLC Films of Different Roughness by Means of Vacuumtribology Accompanied by Mass Spectrometry*, Matthias Kachel,*** Fraunhofer Institute for Mechanics of Materials IWM, Germany

Shot peening prior to deposition allows to effectively create rough DLC coatings and give them a specific topography. While the effect on the coatings adhesion has been discussed earlier, the main objective of this work is to investigate how a strongly increased roughness influences the tribochemistry of hydrogenated diamond-like carbon coatings (a-C:H).

The shot peening treatment was performed on steel bearing rings using globular shot of WC/Co-88/12 with a grain size of 70 µm. By varying the shot peening parameters, different surface topographies were prepared whose relevant parameters as well as spectral information (PSD) were determined using atomic force microscopy (AFM). The tribological experiments were carried out in a vacuum tribometer (ball on disc) that was equipped with a mass spectrometer. Thus, beside the coefficient of friction, the emission of different hydrocarbons and hydrogen for dry and lubricated conditions were detected. The wear of the ball and the coating was measured after the tribological test via profilometry and was then related to the Z-transition of the ball during the experiment. The structural change of the coating was evaluated using Raman spectroscopy.

The investigantions revealed that the signals obtained by the mass spectrometer correlate directly with the chemical composition of the DLC coating and are therefore a measure of gaseous wear. The ratio of gaseous and solid wear was strongly dependent on the particular surface topography which was found to be responsible for the developement of the COF over time. For the lubricated system, gaseous wear originating from the coating and the oil was detected, giving a measure for oil degradation. In total, the friction coefficient was found to be a function of roughness affecting gaseous and solid wear which both influence the chemical transformation of the coating and the formation of a transfer layer.

10:20am **E1-1-8 Plasma-Assisted Lubrication for the Sliding between Polymer and Diamond-Like Carbon***, S Okumura,* Nagoya University, Japan*; T Hibino, **Hiroyuki Kousaka**,* Gifu University, Japan*; N Umehara,* Nagoya University, 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. Recently, DLC is applied to machine parts as coating to reinforce the surface property. On the other hand, the use of polymer parts made of engineering plastics is increasing instead of metal ones because polymer is light, low cost and easily processed. It is expected in the future that the application of DLC to metal comes to be more frequent in order to further improve the sliding property between metal-polymer contact in sliding parts. For that reason, it is important to clarify the characteristic of friction between DLC and polymer. In this research, silicon doped DLC (a-C:H:Si), which is coated by plasma enhanced chemical vapor deposition (PECVD) on a steel disk (SUS304, JIS) 25 mm in diameter, was used as a mating material of sliding against Polyoxymethylene (POM) which is an engineering plastic. Friction tests were conducted in a roller-on-disk apparatus under dry condition, where the side surface of POM roller 5 mm in diameter and 5 mm in height was contacted to DLC-coated disk at a normal load of 1 N. Sliding test was onducted for 20 minutes at a rotation speed of 200 rpm, where the rotation radius of the roller changes from 5.5 to 10.5 mm along the roller axis. During the total sliding distance of 200 m, helium gas flow and helium plasma flow were irradiated for 50 to 100 m, and 100 to 150 m, respectively. Friction coefficient observed for the first 50 m without any irradiation was around 0.2, which was not changed by the following helium gas irradiation. Then, plasma irradiation caused seriously instable and high friction coefficient (around 1.0); however, after stopping the plasma irradiation, the friction coefficient rapidly fell down to around 0.066 and was stabilized. This result indicates the possibility of plasma-assisted lubrication for the sliding between polymer and DLC. (The authors gratefully acknowledge the funding by JST CREST, Japan.)

10:40am **E1-1-9 Integrated Multiscale Material Modelling of Topographical Effects on Wear and Friction in Sliding DLC Contacts***, K Holmberg, A Laukkanen,* VTT Technical Research Centre, Finland*; **Timo Hakala**,* VTT Technical Research Centre of Finland Ltd, Finland*; H Ronkainen,* VTT Technical Research Centre, Finland*; G Stachowiak, P Podsiadlo, M Wolski,* Curtin University, Australia*; M Gee,* NPL National Physical Laboratory, UK*; C Gachot,* Vienna University of Technology, Austria*; L Li,* Hong Kong City University, Hong Kong

In wear studies, surface topography is typically characterized by standard 2D roughness parameters such as R_a and R_q values. These parameters tend to work well with isotropic surfaces but they are not able to provide full information about surface anisotropy and roughness at different scales of measurement. This limitation of commonly used standard parameters is crucial since most real engineering surfaces are anisotropic and multi-scale objects. Computational modelling and simulation of changes occurring in a material due to surface loading, and calculations of stress and strain in loaded contacts is a research area that is rapidly evolving today. Modelling and simulation of a tribocontact help to understand the mechanisms that result in surface cracking, wear particle formation and wear evolution. Numerical simulations can be carried out on several spatial scale levels, from nano size to macro size, by using software representing the material structure from atomic and even sub-atomic to continuum macro and component level.

The effect of surface roughness and topographical orientation on surface stresses influencing wear has been investigated for diamond like carbon (DLC) coated steel surfaces with three levels of surface roughness (R_a) in the range of 0.004 – 0.11 µm, and with topographical orientations of grinding marks (grooves) at 0°, 45° and 90°. A novel multiscale numerical finite element method (FEM) model was developed to integrate the layered and microstructural material features with the orientation of surface topographical features (VTT Propertune). A fractal geometry and surface voxelisation based approach were utilised to derive representative 3D topography. The simulations show the details of the main topographical orientation effects on local stresses affecting wear as they appear at a single scratch by a diamond ball and in a self-mated sliding contact between two rough surfaces. The 45º sliding direction to the grooves resulted in a mixed state of surface loading in contact during the scratch test. The complex state of stress-strain within the roughness peaks decreased the overall tensile stress state and resulted in a greater surface resistance to cracking compared to 0º and 90º directions. Model based calculations showed that the surface structure was about four times more rigid in the direction of grooving compared to the more flexible behaviour in the direction perpendicular to the grooving. This behaviour was confirmed experimentally. The macro-topography had a dominating effect on surface cracking, influencing on both wear and friction, while the micro-topographical features contributed to surface cracking by less than 40 %.

11:00am **E1-1-10 A Comparative Study of Fatigue Properties of TiVN and TiNbN Thin Films Deposited On Different Substrates***, **Hikmet Cicek**,* Erzurum Technical University, Turkey*; O Baran,* Erzincan University, Turkey*; A Keles, Y Totik, I Efeoglu,* Ataturk University, Turkey

Transition metal nitrides, especially ternary phase films attract attention due to its high mechanical and tribological features. Besides these, fatigue properties play a very important role on the performance in service life of these type films. TiVN and TiNbN films were deposited on M2 and H13 steel substrates by reactive magnetron sputtering system. Fatigue properties of the films were characterized via multipass scratch tests. 100, 250 and 500 cycle with two directions multipass tests were conducted at room temperature under the 20 N constant load. Structural properties determined with X-ray diffraction, scanning electron microscopy and energy dispersive spectroscopy. Mechanical features of the films were observed with nano hardness tests. Fatigue behaviors, deformation types, coefficient of frictions of the films and effect of different substrates were discussed comparatively. According to the results, TiNbN films showed much better fatigue resistance than TiVN films although critical adhesion load value of TiNbN was less than TiVN film. TiVN films generally showed brittle type cracks at the edge of the tracks though TiNbN films showed more ductile type cracks. Additionally, the films deposited on M2 substrates exhibited better strength than H13 substrates.

11:20am **E1-1-11 The Mechanical and Tribological Properties of Nanocomposite CrMoSixN Coatings***, **Yu-Chu Lu**, J Duh,* National Tsing Hua University, Taiwan

The CrMoN coatings has been found to have superior mechanical and tribological properties, such as high hardness and low friction due to the solid solution strengthening and the formation of lubricating molybdenum oxide. In this study, the mechanical and tribological properties of CrMoN with various Si content was investigated. With Si contents ranged from 0 at. % to 13.0 at. % , the quaternary $CrMoSi_xN$ coatings were deposited on silicon wafer and Inconel 718 by RF magnetron sputter. Through nanoindentation, the hardness and the H^3/E^{*2} ratio of $CrMoSi_xN$ coatings were obtained. The results showed that mechanical characteristics in $CrMoSi_xN$ coatings were strongly influenced by Si contents. The CrMoSixN coating exhibited highest values in hardness and H^3/E^{*2} ratio with 11.0 at.% Si doped, in which columnar grains turned into nanocomposite structure. The strengthening mechanism of nanocomposite structure was attributed to grain refinement and prevention of direct penetration of cracks. Futhermore, the tribological behavior of CrMoSixN coatings were investigated by ball-on-disc tribometer in atmosphere at room temperature, 500 °C, and 750 °C respectively. The results indicated that the tribological properties of CrMoSixN coatings could be significantly improved with the Si addition due to protective oxide formation on wear tracks and the cooperation of MoO_3 as solid lubricant. At high temperature, MoO_3 contributed to low friction coefficient, while the low wear rate was owing to the presence of SiO_2. With 11 at.% Si doping, the $CrMoSi_xN$ coatings showed superior mechanical and tribological characteristics, leading to potential applications for wearproof and self-lubricating dry cutting tools at elevated temperature.

11:40am **E1-1-12 Comparative Studies on Tribological Behaviors of a Magnetron Sputtered CrSiN Coating Under the Environments of Air and Water***, **Fangfang Ge**, J Congcong, S Tao, L Peng, H Feng,* Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China

Tribological behavior of a magnetron sputtered CrSiN coating with 12.5 at.% Si was studied by ball-on-plate sliding tests in three environments, including air ambient, deionized water, and 3.5 wt.% NaCl water. Then in-situ microscopic examinations on the wear tracks were followed by the combination of scanning electron microscopy (SEM) and a focused ion-beam system. Under the air ambient the coating exhibited a friction coefficient of ~0.47 and a specific wear rate of 1.2×10^{-16} m^3/N m, corresponding to a mild wear process mainly dominated with tribo-oxidation. The tribological behavior of the coating appeared similar features under deionized water and 3.5 wt.% NaCl water. The friction coefficients were relatively lower (~0.24) whereas the specific wear rates increased almost an order of magnitude. It was observed that cracks had formed initially during the running-in period, which might be due to chemical reactions between the coating and the water, resulting more wear of the coating under the environments of deionized water and 3.5 wt.% NaCl water.

12:00pm **E1-1-13 The Mechanical and Tribological Properties of Ti [Nb, V] N Films on the 2024 Al-alloy***, **Ozlem Baran**,* Erzincan University, Turkey*; A Keles,* Ataturk University, Turkey*; H Cicek,* Erzurum Technical University, Turkey*; Y Totik, I Efeoglu,* Ataturk University, Turkey

Al and Al alloys exhibit low wear resistance altough they were used wide range of automobile and aerospace industries. Therefore, in this study, transition metal nitride films were deposited on this light metal alloy in order to improve the wear resistance. The structural properties of the films were analyzed by XRD, SEM and EDS. The hardnesses of the films were determined with a nanohardness test. A pin-on-disc tribometer was used to determine of friction and wear behaviour of the films under different conditions; 50% RH and argon gas. Ti[Nb, V]N films on the Al alloy exhibit a very dense and columnar microstructure. The highest film thickness and the hardness values were obtained as 440 nm and 12 GPa from TiNbVN films. Also, TiNbVN films exhibited the lowest friction coefficent values under different tribo-test conditions. The thickness and the hardness values of TiNbN films are 400 nm and 9.6 GPa, respectively. TiVN films with the lowest thickness (360 nm) and hardness (6 GPa) have the highest friction coefficents under both conditions. The indenter penetration values are 18.75%, 26.4% and 15.23% for TiNbN, TiVN and TiNbVN, respectively. Wear behaviours of the films were affected from the film thickness, hardness and friction coefficent values, significantly.

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