Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room Royal Palm 4-6 - Session E1-1
Friction, Wear, Lubrication Effects, and Modeling

Moderators: Albano Cavaleiro, University of Coimbra, Carsten Gachot, Vienna University of Technology, Nazlim Bagcivan, Schaeffler Technologies GmbH & Co. KG, Germany

8:00am **E1-1-1 Tribologically Induced Oxidation of High-purity Copper as a Function of Sliding Distance***, C Greiner, S Becker,* ***Christian Haug****,* Karlsruhe Institute of Technology (KIT), Germany

Tailoring the surface properties of a material for low friction and little wear has long been a goal of tribological research. Since the microstructure of the material under the contact strongly influences tribological performance, the ability to control this microstructure is thereby of key importance. However, there is a significant lack of

knowledge about the elementary mechanisms of microstructure evolution under tribological load.

In order to under how different elastic and plastic strains influence this microstructure evolution, both were systematically varied in high-purity copper samples. Scanning electron (SEM) and focused ion beam (FIB), electron back scatter diffraction (EBSD) and transmission electron microscopy (TEM) are applied to monitor the resulting microstructure changes.

Our results demonstrate that with increasing strain, the tribologically deformed layer grows deeper into the material. Also an influence on grain rotation and refinement mechanisms will be discussed in the talk.

These results strongly suggest that the amount of tribologically induced strain is a key elementary that needs to be addressed in future modelling of the microstructure evolution in tribological contacts.

8:20am **E1-1-2 Investigation on the Reason for Low Friction between Diamond-like Carbon Coating and Ti-6Al-4V under Fretting Conditions***,* ***Haohao Ding****, V Fridrici, P Kapsa,* Ecole centrale de Lyon, LTDS, France

Ti-6Al-4V / Ti-6Al-4V contacts submitted to fretting (for instance, in the contact between femoral stem and neck adapter in hip joints) present high adhesive wear and very high friction coefficient (around 1.0 – 1.2). Diamond-like carbon (DLC) coatings can be deposited on one of the contacting bodies to decrease friction and wear between two metallic parts in contact.

The objective of this paper is to investigate the reason for the low friction between the DLC coating and Ti-6Al-4V under fretting conditions with a cylinder-on-flat geometry contact. Flats (rough and smooth) and the cylinder (rough) are made of Ti-6Al-4V. Flats were coated with DLC coating using PACVD. The coating thickness is around 2.0 µm. The nano-hardness and the elastic modulus reach 29 ± 4.5 GPa and 236 ± 24 GPa, respectively. Tests were carried out with the normal force of 250 N and the displacement of 20 µm. The evolution of surfaces of both the DLC coating and the Ti-6Al-4V counterbody was explored.

The results indicate that the friction coefficient decreases from around 0.5 to a lower value (around 0.1) during the running-in period, corresponding approximately to the first 100 cycles. After 100 cycles, rotating the cylinder (i.e., putting in contact a new surface from the Ti-6Al-4V counterbody with the already rubbed DLC coating) leads to a new running-in period. Moving the flat (i.e. putting in contact a new surface from the DLC coating with the already rubbed Ti-6Al-4V counterbody surface) results in a continuous low friction coefficient. Those mean that the surface state of Ti-6Al-4V after running-in is the key factor to the low friction. When the DLC coating and Ti-6Al-4V are put into contact, Ti-6Al-4V is adhered to the DLC surface. When the DLC coating starts to slide, more Ti-6Al-4V is abraded and adhered to the DLC. The energy required to break the metallic bonds in Ti-6Al-4V results in the high friction. During the running-in period, the worn surface of Ti-6Al-4V is gradually covered by a tribofilm, which is mainly composed of the worn-off Ti-6Al-4V with oxidization. Carbonaceous material is also observed on the tribofilm. The tribofilm and carbonaceous material separate the Ti-6Al-4V and DLC (impeding direct contact between the 2 counterbodies) and lead to the low friction. Furthermore, the coefficient of friction is higher when the roughness of the coated flat is higher. Cracks of DLC coating are observed on rough flat, but no cracks are observed on smooth flat, because the local contact pressure between asperities from rough flat surface and rough cylinder surface is higher than that between smooth flat surface and asperity from rough cylinder surface.

8:40am **E1-1-3 Tribological and Wettability Evaluation of Magnetron Sputtered WS-C/F Coatings***,* ***Simone Pereira Rodrigues****,* University of Coimbra, Portugal*; S Carvalho,* University of Minho, Portugal*; A Cavaleiro,* University of Coimbra, Portugal

The automotive industry produces a huge amount of mechanical components daily. Namely, the ignition systems need lubrication on their assemblage step, which their excessive use is nowadays a concern because of environmental/human risks. The lubrication tools in use are often stopped for maintenance due to either deficient distribution of the lubricant or high friction phenomena. The solution for these issues is the development of functionalized surfaces addressing both low friction/longer lifetime, due to an improvement of the wear resistance, and further special water/oil wettability properties to improve the lubricant application homogeneity. Two possible surface modification approaches can be used, separately or in synergy, as solutions for those problems: (i) surface structuring by anodization processes and/or (ii) deposition of self-lubricating coatings. In this work, the latter was explored by the optimization of the deposition of self-lubricant coatings based on TMDs, alloyed with carbon and fluorine (W-S-C/F).

WS-C/F coatings were deposited by magnetron sputtering in a reactive Ar/CF_4 gas mixture, from a WS_2 target. Different F contents up to 20 at.% were achieved by varying the CF_4 flow rate. The top-view/cross-section morphologies, the chemical composition/bonding, structure and wettability of the coatings were characterized by SEM, XPS, XRD techniques and water/oil contact angle measurements, respectively. The mechanical properties such as hardness, elastic modulus were as well performed through nanoindentation procedure and the adhesion by scratch testing. The tribological performance was evaluated at room temperature (RT) and at 200 ºC at 20N load against a 100Cr6 steel ball.

The F incorporation led to higher surface hydrophilicity of the coatings, with no effect on the oil wettability, behaviour which could be related to the decrease on the surface roughness. RT tribological tests showed that averagely all tested coatings have similar friction coefficient (COF mean value=0.06), however, both pure WS_2 and the highest F-containing coatings showed a very irregular friction curve at the first 5000 running cycles. Sudden increases of COF, followed by its progressive decrease down to very low values, were observed (0.04 for pure WS_2 and 0.02 for WS-C/F coating). Tribological testing at 200 ºC (dry conditions) showed the same trend, i.e. high F-doped coating reached a COF mean value of 0.016 compared to 0.030 for WS_2 coating. This was interpreted as a beneficial effect of F on increasing the interplanar basal distance of the hexagonal WS_2 tribolayer formed in the contact, decreasing the van der Waals bonding, with the consequent COF decrease.

9:00am **E1-1-4 Tribological Properties and Oxidation Resistance of WN_x Thin Films at High Temperatures up to 500°C***,* ***Daniel Javdošňák****, J Musil, Z Soukup, R Čerstvý, S Haviar, J Houska,* University of West Bohemia, Czech Republic

The paper reports on the structure, microstructure, mechanical properties, friction coefficient µ, wear rate k and oxidation resistance of the WN_x films; here x=N/W is the stoichiometry of nitride films. The films were reactively sputtered from a W target of diameter of 100 mm on Si(100) and Steel 15330 substrates in a mixture of $Ar+N_2$ gases using an unbalanced magnetron powered by the AC pulsed power supply. The properties of sputtered WN_x films were characterized by (i) X-ray diffraction (XRD), (ii) Scanning Electron Microscope (SEM), (iii) micro–indentation testing, (iv) pin–on–disk tribometry in wide range of temperatures T from room temperature (RT) up to 500°C and (v) ellipsometry. It was found that sputtered WN_x films are polycrystalline nanocomposites composed of either a mixture of low–T α-W and high–T β-W_2N the phases at x≤0.5 or high–T β-W_2N and low–T δ-WN the phase and exhibit: (1) high values of the hardness H, effective Young's modulus E^*, elastic recovery W_e increasing with increasing x up to 34 GPa, 0.13 and 88%, respectively, (2) the friction with Al_2O_3 ball (i) increases from 0.3÷0.4 at RT to 0.8÷1.2 at 200°C and (ii) decreases to 0.5÷0.6 at 400°C and sliding distance of 1000 m, (3) the wear with Al_2O_3 ball increases from 10^{-8} mm^3/Nm at T≤200°C up to $\sim 2.5\times10^{-6}$ mm^3/Nm at T ranging from 200 to 400°C. The WN_x films are completely removed from the substrate at T=500°C already at sliding distances of about 350 to 600 m due to formation of the WO_x scale on the coating surface.

9:20am **E1-1-5 Correlation between Evolution of Roughness Parameters and Micropitting of Carburized Steel Surfaces under Boundary Lubrication Condition**, ***Sougata Roy***, *D White, S Sundararajan,* Iowa State University, USA

This paper investigates the correlation between the evolution of the amplitude (R_a, R_{RMS}, R_{sk} and R_{ku}) and spatial (autocorrelation length) roughness parameters and micropit initiation and propagation during rolling contact fatigue (RCF) of carburized steel samples under boundary lubrication conditions. Steel samples with three levels of retained austenite or RA (~0%, 15% and 70% as measured by micro X-ray diffraction) were prepared for the RCF study which was conducted with a rolling-sliding contact in a micropitting rig. It was observed that run-in happened within an order of 10^4 cycles for all samples and during this period, a significant decrease in R_a and R_{RMS} occurred while the correlation length increased and stabilized. The low RA samples failed due to early crack initiation and rapid crack propagation. The medium and high RA samples showed initiation and propagation of micropitting during RCF life. Micropitting initiation and propagation were captured for the mid and high RA samples using an optical profilometer which utilizes a non-contact white light interferometry technique. Micropitting trends were then correlated with different surface roughness parameters. It was observed that, if surface change due to mechanisms other than micropitting is controlled, then R_a and R_{RMS} follow the same trend with the propagation of micropitting. Skewness can be used as a parameter to predict the initiation and propagation of micropitting; significant propagation resulted in a decreasing trend of skewness (negative) and increasing trend of kurtosis. Transverse directional correlation length also was found to be in agreement with the propagation of micropitting. It was observed that the correlation length decreased as micropitting progressed. The present study shows that drivetrain industries can track correlations with surface roughness parameters to predict the long-term performance of the components under the boundary lubrication regime.

9:40am **E1-1-6 The Influence of Temperature on the Wear Mechanisms of a Cobalt-based Alloy Contact Subjected to Fretting: from an Abrasive Tribo-oxydation Process to the Glaze Layer Response**, ***Alixe Dreano***, *S Fouvry, G Guillonneau,* LTDS - Ecole Centrale de Lyon, France

Cobalt-based alloys are widely used in the aeronautical industry for their good mechanical properties and corrosion resistance at high temperature. Vibrations, or other micro-displacements, of mechanical pieces initiate fretting and then lead to wear. Wear mechanisms of cobalt-based alloys are commonly known to be dependent on temperature. Above a transition temperature TGL, wear rate decreases and becomes very low given that a compacted and oxidized layer is spontaneously created in the contact ("glaze layer"). Below TGL, wear is severe and the tribolayer is not generated. The high-temperature layer has been thoroughly studied by many authors who associated its formation to the capacity of oxidized debris to sinter and adhere to the bulk metal.

The present study was focused on the change of wear mechanisms occurring through a range of temperatures (from ambient to 600°C). A cross-cylinders cobalt-based alloy against alumina contact was subjected to gross-slip fretting. The study showed that wear, before severe-to-mild wear transition, TGL, is controlled by the continuous oxidation of the interface and is therefore strongly influenced by the operating temperature and frequency of solicitation. An analytical wear law was developed in order to describe the wear mechanism below TGL. The dependence of TGL on frequency was also outlined and associated to the capacity of debris to sinter. Finally, to completely describe the behavior of the tribocouple, the mechanical response of the glaze layer is discussed in the light of the results of in-situ compression of micro-pillars cut into the glaze layer.

10:00am **E1-1-7 Coated Surface Wear Resistance Design by Comutational Modelling**, ***Kenneth Holmberg***, *A Laukkanen, T Hakala,* VTT Technical Research Centre of Finland Ltd, Finland **INVITED**

The presentation gives an overview of Integrated Computational Materials Engineering (ICME) and the approach and techniques we have used for computational materials modelling and simulation. The focus is on meso- and microscale modelling, integrated approaches and wear related applications. The FEM modelling technique has been stretched to observe stress and fracture phenomena on microscale in thin hard diamond-like carbon (DLC) and titanium nitride (TiN) physical vapour deposited coatings and an equation was developed to show the dominating effects on potential wear failure.

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. 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. Modelling and simulation of a tribocontact help to understand the mechanisms that result in surface cracking, wear particle formation and wear evolution and to work out guidelines for optimal contact and surface design for best friction and wear performance tailored for specific applications. 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. VTT has introduced the *VTT Propertune* approach and software to find optimal solutions to industrial material challenges worldwide (http://www.vttresearch.com/propertune).

10:40am **E1-1-9 Room and Elevated Temperature Sliding Wear Behavior and Mechanisms of a Cold Sprayed Ni-WC Composite Coating**, ***Tyler Torgerson***, *M Harris,* University of North Texas, USA; *S Alidokht,* McGill University, Canada; *T Scharf, S Aouadi,* University of North Texas, USA; *R Chromik,* McGill University, Canada; *J Zabinski,* Army Research Laboratory, USA; *A Voevodin,* University of North Texas, USA

Cold sprayed Ni-WC metal matrix composite coatings have advantageous tribological properties that have only been investigated in the literature at room temperature. This study sought to identify their elevated temperature dry sliding behavior from room temperature up to 400 °C as well as during thermal cycling with a sliding speed of 2 cm/s and a load of 2.45 N. Further characterization included the use of SEM, EDS, XRD, XPS, Raman spectroscopy, interferometry, and hardness measurements. Results indicate that an increasing temperature leads to a decrease in friction and an increase in wear. The coefficient of friction decreased from 0.41 at 23 °C to 0.32 at 400 °C, while the wear rate increased from 0.47×10^{-4} mm^3 N^{-1} m^{-1} at 23 °C to 3.67×10^{-4} mm^3 N^{-1} m^{-1} at 400 °C. This lowering of friction is attributed to the formation of a lubricious tribochemical phase in the wear track. The increase in wear is due to a combination of thermal softening and a change in the wear mechanism from adhesive to abrasive. During thermal cycling, the coating exhibited self-adaptive behavior from the high to low friction regime. The results revealed that thermal softening and tribochemical reactions that occurred at elevated temperatures slightly compromised the wear resistance while producing a lubricious tribofilm. Therefore, WC-Ni cold spray coatings are potential candidates for elevated temperature sliding wear applications.

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