Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room Town & Country B - Session E1-1-TuA
Friction, Wear, Lubrication Effects, and Modeling I

Moderators: Noora Manninen, Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein, **Andreas Rosenkranz**, Andreas Rosenkranz, Universidad de Chile

1:40pm **E1-1-TuA-1 2D Transition Metal Carbide MXenes: Their Synthesis, Tunable Compositions and Mechanical Properties***, **Babak Anasori (banasori@iupui.edu)**,* Indiana University-Purdue University , USA*; B. Wyatt,* Indiana University-Purdue University, USA **INVITED**

Two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides, known as MXenes, have evolved as competitive materials and fillers for developing composites and hybrids for different applications. MXenes are denoted by a chemical formula of $M_{n+1}X_nT_x$ (n = 1 to 4), where M represents n+1 layers of early transition metals (groups 3 – 6 of the periodic table) which are interleaved by n layers of X, where X represents carbon or nitrogen. In addition, T_x represents surface terminations bonded to the outer M layers of MXenes, where T are generally a mixture of –O, –F, –(OH), or –Cl surface groups. MXenes are synthesized via a top-down topochemical etching of their precursor carbides and nitrides, such as MAX phases. MXene flakes have strong mechanical properties (330 ± 30 GPa and 386 ± 13 GPa for $Ti_3C_2T_x$ and $Nb_4C_3T_x$, respectively), which make MXenes the stiffest solution-processable 2D nanomaterials to date. The current forty synthesized MXene compositions paired within-depth ability to control their composition and structure makes MXenes a unique family of 2D materials with unlimited number of compositions and tunable properties. In this talk, we provide an overview of different MXenes compositions, their synthesis, and MXenes' mechanical properties and discuss the effects of MXenes' compositions, synthesis, and processing steps on their mechanical properties.

Keywords: MXenes, 2D materials, carbides, mechanical properties, composites.

2:20pm **E1-1-TuA-3 Grain Boundary Sliding and Low Friction in BCC Metals***, **Michael Chandross (mechand@sandia.gov)**,* Sandia National Laboratories, USA*; A. Hinkle,* CCDC & CBC, Aberdeen Proving Ground, USA*; M. Jones, P. Lu,* Sandia National Laboratories, USA*; N. Argibay,* Ames Laboratory, USA **INVITED**

We show evidence of low friction in BCC metals through molecular dynamics simulations and ultra-high vacuum experiments. This is shown to be correlated with grain boundary sliding (GBS) as the primary mechanism of deformation. Specifically, when grain sizes at the sliding interface are smaller than a critical, material-dependent value (on the order of 10-30 nm), a crossover occurs from dislocation mediated plasticity and Hall-Petch strengthening to GBS and interfacial softening. Results from simulations and experiments are quantitatively compared to a new predictive model of shear strength.

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3:00pm **E1-1-TuA-5 Evaluation of Tribocoatings in Low Viscosity Fuels***, **Maddox Dockins (maddoxdockins@gmail.com)**, A. Ayyagari, S. Srivilliputhur,* University of North Texas, USA*; S. Berkebile,* US DEVCOM Army Research Laboratory, USA*; D. Berman, A. Voevodin, S. Aouadi,* University of North Texas, USA

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Degradation of sliding surfaces creates a significant problem for mechanical assemblies. In the case of next generation fuel delivery systems, steel on steel contacts in low viscosity fuel environments have been shown to experience scuffing failure after extended operation under rough conditions, as well as poor general tribological performance. To prevent this scuffing-induced failure, various surface modification techniques were implemented, such as the application of carbide- and nitride-based protective coatings via PVD and plasma spray methods. These surface modification techniques were evaluated in various fuel environments and counterbody compositions using a high frequency reciprocating rig tribometer in a sliding velocity range of 0.2 to 0.6 m/s and contact pressures ranging from 500 to 1200 MPa. Their relative performance was evaluated according to their wear rates, average coefficient of friction, and oxidation as determined via SEM/EDS. These results were explained theoretically through density functional theory calculations that quantify the effect of surface interactions with the fluid.

4:00pm **E1-1-TuA-8 Phototribology: Control of Friction by Light***, B. Perotti,* UCS, Brazil*; A. Cammarata,* Czech Technical University in Prague, Czech Republic*; F. Cemin,* Université Paris-Saclay and UNICAMP, Brazil*; S. Sales de Mello,* UCS and UNICAMP, Brazil*; L. Leidens,* UCS, Brazil*; F. Echeverrigaray,* UCS and UNICAMP, Brazil*; T. Minea,* Université Paris-Saclay, France*; F. Alvarez,* UNICAMP, Brazil*; A. Michels,* UCS, Brazil*; T. Polcar,* University of Southampton and Czech Technical University , UK*; **Carlos Figueroa (cafiguer@ucs.br)**,* UCS, Brazil

Friction phenomenon is a complex manifestation of nature originated in energy dissipation events owing to the mechanical lost work of non-conservative forces. It is a property influenced by contact area, normal force, surface chemistry, mechanical properties, among others. There are several ways of tuning friction, all of them nonreversible processes. Thus, the active control of friction though external sources is a challenge in tribology. In this study, we report active control of friction forces at the nanoscale in TiO_2 thin films (anatase) obtained by HiPIMS as a function of the presence or absence of UV radiation (λ = 365 nm and nominal power of 5 mW) by friction force microscopy (FFM). According to the effects, this phenomenon of light-matter interaction is reversible, stable, and can be tuned/controlled by UV light. The radiation incidence modifies the physicochemical interactions at the sliding interface in TiO_2 thin films bringing on a dramatic reduction of frictional force of up to 61%. To understand the energy dissipation process, the characteristic frequencies of the system were analyzed; to this aim, atomic force microscopy signals were measured by wavelet analysis. The results show that the surface activation by UV light reduces the dissipated energy. *Ab initio* simulations were used to corroborate that the electron excitation augments the electronic density on the material surface. According to these results one can conclude that the reduction in friction is a result of the lower atomic orbital overlapping on the surface. These findings contribute to a new conceptual framework in tribology where light may be defined as a fourth body and the integration of tribology with photonics and optoelectronics providing a promising direction for applications in micro- and nano-opto-electromechanical systems.

4:20pm **E1-1-TuA-9 Development and Evaluation of Self-Lubricating Nanocomposite Coatings for Metal Forming Dies***, **Jianliang Lin (jlin@swri.org)**,* Southwest Research Institute, San Antonio Texas, USA

Die failure in metal forming industry results in substantial losses of time and money. Conventional lubricants are widely used for die release as well as for cooling assistance on the die surface. However, lubrication is difficult at high temperatures. Oxidation and scaling occur on the work pieces that lead to poor surface finish and possible warping of the material during cooling. The aim of the research is to develop a self-lubricating nanocomposite coating system for metal forming die components and investigate the self-lubricating behavior and thermal stability of the coatings at elevated temperatures. The designed coating systems consist of a nanocomposite matrix doped with solid lubricant phases, e.g. noble metals and amorphous carbon. The composite structure offers multifunctionality, including high wear resistance, good oxidation resistance, crack resistance, and self-lubricating properties at elevated temperatures. In this study, different nanocomposite coating matrixes, e.g. TiSiCN and CrAlN, were doped with different levels of Ag. The coatings were deposited by high power impulse pulse magnetron sputtering (HiPIMS) assisted by hot filaments. The elemental composition, phase structure, microstructure, adhesion, and mechanical properties of the coatings were studied by different means. The tribological properties and self-lubricating behavior of the coatings were evaluated using a high temperature tribometer at 700 °C. The thermal stability and thermal shock resistance of the coatings were evaluated using thermal cyclic test by cycling the coatings from RT to 700 ^{o}C with a testing cycle up to 1200 cycles. The results showed that the density and adhesion of all coating systems decreased as the Ag content increased in the coatings. The lowest COF of 0.1 was achieved in the coatings at 700 ^{o}C. Excellent thermal stability and thermal shock resistance, and high temperature lubricity were observed in the coatings with an optimal Ag content.

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