Advanced Surface Engineering Division
Room C123 - Session SE+TF-MoA

Mechanics and Tribology of Thin Films and Coatings

Moderators: Rebecca Cai, Virginia Tech, **Suneel Kumar Kodambaka**, Virginia Tech

1:40pm **SE+TF-MoA-1 Mini-Module Stress Testing to Assess 'Fatigue-Like' Failure Mode of Gridlines on Silicon Solar Cells***, A. Chavez, **Sang Han**,* University of New Mexico*; S. Huneycutt, A. Ebong,* University of North Carolina at Charlotte*; D. Harwood, N. Azpiroz,* D2Solar

Microcracks in solar cells can eventually propagate through metal gridlines and busbars, leading to PV module power loss over time. With the latest glass/glass PV module construction – in which the glass is only heat-treated (not tempered) and its thickness is reduced from 3.2 mm to 2.0 mm – along with ever-increasing module size, the stress-induced cell cracks are rapidly becoming one of the main degradation modes. In this study, we compare how metal matrix composite gridlines fare in comparison to standard silver gridlines against three-point-bending stress test. We have fabricated two-cell, mini-modules with full-size Passivated Emitter and Rear Contact (PERC) cells. The backside of each cell is laser-scribed prior to encapsulation to initiate cell cracks. The completed mini-modules are then placed on a three-point-bending setup and flexed until the cells crack, and the cracks propagate through the gridlines to cause electrical discontinuity. The mini-modules are then subjected to cyclic mechanical stress on the three-point-bending setup up to the sub-critical fracture stress level to simulate the field operation and to characterize the long-term 'fatigue-like' wear-out failure. The results show that enhanced ductility and compliance of composite gridlines lead to their increased durability compared to standard silver gridlines, strongly suggesting increased lifetime of PV modules against cell cracks.

This material is based upon work supported by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) under the Solar Energy Technologies Office Award Number DE-EE0009013.

2:00pm **SE+TF-MoA-2 Relating Stress in Thin Films to the Underlying Kinetic Processes: Experiments and Modeling***, E. Chason, **Tong Su**,* Brown University

Stress in thin films can have a significant impact on their performance and reliability.Since stress is affected by many parameters (growth rate, temperature, microstructural evolution, composition, particle energy for sputter deposition, etc.), a fundamental understanding of its origins stress would allow it to be predicted and optimized.We describe a model for we have developed to explain stress evolution during deposition in terms of the underlying kinetic processes. The model includes mechanisms related to non-energetic growth kinetics, microstructural evolution and energetic particle bombardment.Examples are discussed that use the model to explain the dependence of stress on the growth rate, grain growth kinetics and sputter pressure.A user-friendly computer program based on the model is described that is available to interested users to analyze wafer curvature measurements.

2:20pm **SE+TF-MoA-3 Tailoring the Tribocorrosion Resistance of Al-based Metallic Thin Films via Alloying and Nanolayering***, **Wenjun (Rebecca) Cai**,* Virginia Tech **INVITED**

The increasing complexity and severity of service conditions in areas such as aerospace and marine industries, nuclear systems, microelectronics, batteries, and biomedical devices etc., imposes great challenge on the reliable performance of metallic thin films subjected to simultaneous surface stress and corrosion. However, the design of strong and corrosion-resistant coatings, especially those containing passivating elements such as Al are challenged by the tradeoff between strength and corrosion resistance. Towards this end, this talk will focus on the development of novel microstructure design strategies for metallic thin films to mitigate the combined attack of wear and corrosion (i.e. tribocorrosion) under harsh conditions. Two design strategies will be discussed to overcome this long-standing dilemma: by forming solid solution alloys and nanostructured multilayers. These studies provide insights for general design guidelines to engineer more robust, high-performance metals for use under harsh conditions.

3:00pm **SE+TF-MoA-5 Tribological Properties of Conversion Layers and Carbon-based PVD Coatings for Rolling Bearing Applications***, **Esteban Broitman**, A. Ruellan, R. Meeuwenoord, D. Nijboer,* SKF B.V. - Research and Technology Development, Netherlands

In this study, different coatings and conversion layers have been compared in terms of friction performance based on a single-contact oil-lubricated tribometer and on a grease-lubricated double row bearing friction test rig ran under relevant operating conditions for a railway application. Conversion layers like zinc-calcium-phosphate, manganese-phosphate and black-oxide have been compared on friction performance to that of an un-coated steel surface and to a proprietary diamond-like-carbon base coating.

Results demonstrate that the optimum conversion layer can reduce friction by more than 25% on rolling/sliding raceway contacts (ball-on-disk) and up to 80% on the sliding flange contacts (roller-on-disk), which share a significant portion of power losses in roller bearing units. Results at the bearing level demonstrate that the same optimum conversion layer can reduce the running torque by approximately 30% compared to the current products both at low and intermediate speeds relevant to intercity trains.

3:20pm **SE+TF-MoA-6 The Tribological Behaviour of TiAlN Coating Under High-Temperature Conditions***, **Aljaž Drnovšek**,* Jozef Stefan Institute, Slovenia*; P. Šumandl,* Faculty of Natural Sciences and Engineering, University of Ljubljana, Slovenia*; Ž. Gostenčnik,* Jozef Stefan Institute, Slovenia*; M. Čekada,* jozef Stefan Institute, Slovenia

TiAlN coating is a popular hard coating for high-temperature applications such as high-speed cutting and cutting of new, hard-to-cut materials. However, the most commonly used method for depositing this coating on cutting tools, cathodic arc evaporation, can result in a relatively rough surface due to the emission of micro-droplets. This roughness and the presence of embedded droplets in the coating matrix can significantly affect the coating's wear and friction properties

Our objective was to assess the wear and friction properties of the TiAlN coating during both the running-in and steady-state periods under varying temperature conditions. To evaluate the performance of the TiAlN hard coating, we conducted tribological tests using a high-temperature pin-on-disc tribometer. The tests were carried out with an Al_2O_3 ball as a counter body at different temperatures: room temperature, 250 °C, 500 °C, and 700 °C. We varied the test duration at specific temperatures, ranging from 50 up to 140,000 cycles, to examine the effect of test length on the coating's wear and friction properties. After each tribological test, we analysed the coatings.

The results indicated that the coating experienced the highest wear during the room temperature test. Conversely, the wear during the running-in phase and steady-state friction was the lowest at 250°C. As the temperature increased, the wear rate rose, which we attributed to tribo-oxidation and fatigue caused by the high test lengths. Ultimately, the coating delaminated from the WC-C substrate at the highest temperature. The asperities on the surface of the coating due to micro-droplets played a significant role in friction and wear behaviour, as they were a primary source of wear particles and the first spots of oxidation on the coating.

We conducted detailed 3D profilometry, SEM and FIB analyses on numerous samples to determine the wear mechanisms at different stages of high-temperature wear. In addition to tribological evaluation, we performed high-temperature mechanical tests at the same temperatures as the tribological tests.

The combination of these analyses allowed us to gain a comprehensive understanding of the wear mechanisms and behaviour of the TiAlN coating at high temperatures. By analysing the samples at different stages of wear, we were able to identify the dominant wear mechanisms and how they evolved over time.

4:00pm **SE+TF-MoA-8 Atomic Layer Deposition Coatings on Micron-Sized Iron Powders for Increased Oxidation Resistance***, **Chris Gump**, J. Burger, T. Porcelli, J. Travis, B. Boeyink, T. Champ,* Forge Nano

The physical, electrical, and magnetic properties of micron-sized and smaller metal powders make them useful for a variety of applications, including additive manufacturing, electronic components, metal injection molding, microwave absorption, and powder metallurgy. As the particle size of these metals becomes smaller, oxidation of the particle surface becomes a larger issue. In the case of flammable metal powders like iron and titanium, this can have severe safety implications, as the rapid oxidation of the powder can result in a metal fire or dust explosion. However, even the slower oxidation reactions that occur in salty, foggy, or typical ambient conditions can reduce shelf life and have other negative effects on the properties of products made from these feedstocks. The desirable properties of these materials can be preserved by encapsulating the powders with a barrier film. To minimize the effects on the properties of the composite particles, the barrier film should be as thin as possible.

Atomic Layer Deposition (ALD), long used in the semiconductor industry for coating wafers, has in recent years been applied to a wider range of application spaces, including the surface modification of powders with nanometer-scale films. We studied the deposition of thin, nanoscale alumina ALD barrier films onto metal powders, using carbonyl iron powder (CIP) as a model substrate that has a range of applications.Coatings were performed on 30 g batches of powder in a highly scalable fluidized bed reactor. The barrier properties of the films were studied as a function of deposition temperature (80 – 230°C) and film thickness (1 – 8 nm), using thermogravimetric analysis in oxygen as the performance metric. Optimal barrier performance, in terms of the shift in onset temperature for oxidation, occurred for the middle range of deposition temperatures. The thickest films were able to shift the onset temperature for oxidation by as much as 300°C (from 250°C to 550°C). The barrier performance as a function of temperature was found to correlate with previously published studies of the film density and growth per cycle (GPC) of Al_2O_3 ALD deposited as a function of temperature.Although not characterized in this case, the barrier films are also expected to decrease electrical conductivity while maintaining magnetic susceptibility. The deposition process has been successfully demonstrated at the 1-5 kg scale, and the 100 kg scale for similar metal powders, with the potential for even higher throughputs on established coating tools.

4:20pm **SE+TF-MoA-9 Characterizing the Composition, Structure, and Mechanical Properties of Titanium Silicon Nitride Erosion Resistant Coatings***, **Gilad Zorn**, P. Shower, S. Weaver, R. Rose, J. Her, J. Salisbury,* GE Research Center

Titanium nitride (TiN) coatings have a wide range of applications due to their practical properties such as high hardness, good corrosion resistance, heat resistance and excellent wear resistance. They have been widely used in various industries including decorative coatings, diffusion barriers and hard coatings. The properties of TiN can be greatly enhanced by addition other elements, such as Si [1-2]. Incorporation of Si in the TiN cubic structure leads to formation of TiSiN coatings characterized by high hardness and high oxidation resistance up to 800 °C. This enables synthesizing coatings and designing materials with a broad range of applications, especially as materials that should perform under harsh environments. The ternary TiSiN system is formed due to the total miscibility of Si, which creates a solid solution while preserving the crystalline structure B1 of TiN. Si is also believed to create nanocomposite structure of TiSiN coatings consisting of nanocrystalline TiN grains encapsulated by an amorphous silicon nitride (Si_3N_4) matrix.To achieve high hardness TiN films, significant bonding strength between Ti and N must be achieved.If the bonding is too weak, the surface of the coating can oxidize, forming titanium oxynitride and eventually TiO_2 even at room temperature conditions [3]. The oxynitride and oxide forms are known to exhibit a lower hardness than TiN and experience oxidation propagation.

This study is focused on the characterization of TiSiN hard coatings. For example, X-ray Photoelectron Spectroscopy (XPS) was used to study the compositions and high resolution XPS was used to determine the surface oxide to nitride ratios. Mechanical tests were performed with nano indenter to determine the hardness of these coatings. Figure 1 shows the correlation between the hardness of the films and the percentage of the XPS titanium oxide component.X-ray diffraction confirmed the formation of titanium nitride cubic phase and different crystallographic orientations were observed depending on the composition of each film. The results of this study show that adding Si and reducing the oxygen level improved the performance of the nitride films as erosion resistant coatings.

1. Akhte, Rumana; Zhou, Zhifeg; Xie, Zonghan, Munroe, Paul *Surface and coating technology* 425 (2021) 127687.
2. Greczynski, G.; Bakhit, B.; Hultman, L.; Odén, M. *Surface and coating technology* 398 (2020) 126087.
3. Logothetidis, S.; Meletis, E.I.; Stergioudis, G.; Adjaottor, A.A. *Thin Solid films* 338 (1999) 304.

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