Thursday Afternoon, April 23, 2026

Plasma and Vapor Deposition Processes
Room Palm 1-2 - Session PP4-ThA

Greybox Models for Wear Prediction

Moderators: Philipp Immich, IHI Hauzer Techno Coating B.V., Netherlands, **Ludvik Martinu**, Polytechnique Montréal, Canada

2:00pm **PP4-ThA-3 End-to-End Prediction of Coating Properties and Film Distribution via a Digital-Twin Framework***, **Adam Obrusnik [obrusnik@plasmasolve.com]**, Krystof Mrozek, Kristina Stastna, Petr Zikan,* PlasmaSolve s.r.o., Czechia **INVITED**

Physical vapor deposition (PVD) and plasma-enhanced chemical vapor deposition (PECVD) processes generate vast streams of sensor data, waveforms, and post-coat metrology, yet only a small portion of this information informs engineering decisions. This work presents PlasmaSolve's **hybrid digital-twin framework**, a *greybox* approach that combines physics-based plasma and transport simulations with machine-learning models trained on process logs, diagnostic data, and coating metrology. The framework is implemented within the MatSight simulation ecosystem.

The framework enables **end-to-end prediction of key coating properties**, including **film composition, thickness, and their spatial gradients**, as well as **hardness, roughness, or residual stress** - all derived directly from the coating recipe and coating tool layout. These quantities are resolved over complex 3D substrate geometries using the MatSight 3D Uniformity App to produce full-field maps of **mass and energy flux distributions**, linking plasma behavior to the resulting film structure and uniformity.

While the presented models do not directly predict wear progression, they capture the **precursor variables that govern wear performance**, such as local variations in stoichiometry, microstructure, and residual stress. This capability bridges a critical gap between process conditions and the mechanical stability of coatings under service environments. Case studies demonstrate how the hybrid digital twin reduces experimental trial runs by up to **90 %**, accelerates recipe transfer between coating tools, and improves the reproducibility of wear-relevant coating metrics.

The talk outlines the architecture of the greybox framework, emphasizing how simulation-derived features enhance extrapolation beyond the training domain. It concludes with perspectives on extending this approach toward **direct wear and lifetime prediction**, forming a foundation for data-driven process optimization and reliability assurance in advanced thin-film manufacturing.

2:40pm **PP4-ThA-5 Influence of Temperature- Dependent Mechanical Properties on Tool Load in Cutting***, Christian Kalscheuer, Kirsten Bobzin,* ***Xiaoyang Liu [liu@iot.rwth-aachen.de],*** Surface Engineering Institute - RWTH Aachen University, Germany*; Benjamin Bergmann, Berend Denkena, Nico Junge,* Institute of Production Engineering and Machine Tools, Hannover, Germany

Hard physical vapor deposition (PVD) coatings are widely applied to protect cutting tools against wear. Simulating the thermomechanical load of coated tools is an important approach to understand wear mechanisms. In previous studies, the PVD coating in finite element chip formation simulations has typically been treated as a rigid body, or its properties were assumed to remain constant in the simulation. However, the mechanical properties of PVD coatings vary with temperature during cutting. Assuming constant properties may therefore reduce simulation accuracy. In this study, the temperature-dependent mechanical properties of a TiAlCrN coating are determined using high temperature nanoindentation, while thermal diffusivity is measured at different temperatures using the laserflash method. These experimentally determined coating properties were integrated in the simulation for the coating. Based on the experimental results the thermomechanical load is then simulated for cutting of C45 steel in a finite element chip formation simulation. The study compares the results of temperature-dependent mechanical coating properties with constant properties. The results show that simulations with temperature-dependent coating properties are different to simulations with fixed coating properties. This represents an advance in the research direction of understanding the thermomechanical tool load during cutting.

3:00pm **PP4-ThA-6 Discovering Hard, Conductive Films via Combinatorial High-Throughput Multimodal Characterization and Machine Learning***, **Brad Boyce [blboyce@sandia.gov]**,* Sandia National Laboratories, USA **INVITED**

Hard, electrically conductive films with low friction and high wear resistance are relevant to electrical contact applications. Here we augment traditional process-structure-property investigations with an accelerated workflow to detect material structure/composition, prognose associated properties, and adapt the associated process to achieve improved product outcomes.This accelerated detect-prognose-adapt cycle is aided by four key elements: (1) automated combinatorial synthesis to enable rapid parameter sweeps, (2) high-throughput evaluation of both conventional and surrogate indicators of material chemistry, structure, and properties, (3) machine learning algorithms to unravel correlations in high-dimensional spaces beyond expert cognition, and (4) batchwise Bayesian optimization strategies to balance efficient exploration and exploitation.Unlike other ML-driven materials exploration campaigns that focus on variations in the composition of the material, here our primary emphasis is on variations in deposition conditions.We identify particular deposition conditions that produce metallic thin films with exceptional hardness (>9 GPa), low friction (m<0.1), and low electrical resistivity on par with commercial electrical contact alloys. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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