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

Greybox Models for Wear Prediction

Moderator: Philipp Immich, IHI Hauzer Techno Coating B.V., Netherlands

1:40pm **PP4-ThA-2 Integrating Tribological Descriptors and Physics-Informed Modelling for Tool Wear Prediction in PVD Coated Milling Tools***,*
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Accurate prediction of tool wear in milling remains a major challenge due to the complex interplay between process parameters, coating properties, and local tribological phenomena at the cutting interface. Conventional approaches, whether based on extensive machining experiments or purely data-driven algorithms, often struggle to generalise across coatings and lack physical interpretability. This work includes a descriptor from tribological tests that connects generalised wear characteristics obtained through streamlined, indicative testing protocols, yielding a concise, physics-oriented model that flexibly adjusts to changes in operational parameters and contextual influences.

Building on this foundation, a hybrid model is introduced that merges the descriptor with process variables and perspectives derived from numerical simulations, thereby creating a more comprehensive depiction of wear evolution that aligns empirical patterns with conceptual frameworks. Predictions involving the range of coating variants (pulsed DC to HiPIMS) confirm the descriptor's ability to mirror the wear results from the real-world milling experiments. In essence, this approach establishes a flexible, understandable platform for wear forecasting applicable across diverse tool setups and everyday workpieces, dramatically reducing reliance on resource-intensive testing and characterisation.

2:00pm **PP4-ThA-3 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.

2:40pm **PP4-ThA-5 Influence of Temperature- Dependent Mechanical Properties on Tool Load in Cutting***,*
Christian Kalscheuer [kalscheuer@iot.rwth-aachen.de], *Kirsten Bobzin, Xiaoyang Liu,* 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.

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