Monday Afternoon, May 12, 2025

Plasma and Vapor Deposition Processes
Room Palm 3-4 - Session PP6-MoA

Greybox Models for Wear Prediction

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

1:40pm **PP6-MoA-1 Greybox Models for the Qualification of Coated Tools for High-Performance Cutting**, ***Kirsten Bobzin [info@iot.rwth-aachen.de]***, *Christian Kalscheuer, Muhammad Tayyab, Xiaoyang Liu,* RWTH Aachen University, Germany **INVITED**

The real application behaviour of coated cutting tools cannot be satisfactorily described mathematically. The incipient failure, wear progression and remaining service life cannot be predicted. However, there is a solid basic knowledge in machining technology and materials engineering, which is being described more and more fundamentally and atomistically in the form of white box models. This includes numerical simulations, which are becoming increasingly computationally and time intensive as the level of detail increases. However, the highly non-linear interactions of reality can never be fully described due to idealized assumptions. In contrast, black box models of machine learning can model complex correlations with a sufficient database and are capable of learning. However, physical interactions are then often not understood and their robustness in relation to changing boundary conditions remains uncertain.

As a new research approach, the existing deterministic white box models are to be combined with new data-driven black box models in grey box models. The robust but inaccurate predictions from white box models will be converged into a precise target window using data-driven and adaptive black box models. Already existing machine learning algorithms form the solution space for this. The gap that currently exists between stationary material properties before and after use, i.e. the unsteady system behaviour of coated tools during machining, is being researched and closed. This should enable knowledge-based selection and qualification of coated tools for more efficient machining processes in the future.

The large amounts of data collected but largely unused in research are seen as key. On the materials engineering side, the coated tools are initially analysed in their manufacturing state. However, the focus here is much more on time-dependent changes due to thermal, mechanical, and chemical loads during machining. The stress collective in the machining process is increasingly being monitored in situ in the form of forces, temperatures, images, or noises. The aim is to be able to trace changes in the in-situ measurement data back to the damage progress of the tools. Initially heterogeneous data formats from the machining process and from materials analysis need to be combined. As much real data as possible is systematically recorded, qualified, and correlated. The valid interpretation of the results requires a holistic view of the entire service life and interdisciplinary cooperation.

2:20pm **PP6-MoA-3 A Grey-Box Modell for Predicting Friction Coefficients of Coated Cutting Tools for Improved Wear Modelling**, ***Jan Wolf [jan.wolf@ifw.uni-stuttgart.de]***, University of Stuttgart - Institute for Machine Tools, Germany*; Nithin Kumar Bandaru, Martin Dienwiebel,* Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany*; Hans-Christian Möhring,* University of Stuttgart - Institute for Machine Tools, Germany

Wear of cutting tools is known to affect the surface integrity of the workpiece and contributes significantly to machine downtime. It has been shown that the wear rate increases dramatically once the coating is worn through. Predicting the wear of the coating is therefore a good indicator for the remaining useful life. Although white-box models based on Finite Element Analysis exist and showed good wear prediction capabilities for uncoated tools, transferring this approach to only model wear of coatings is challenging. One of the main factors for precise wear modelling is to use a precise friction model which captures the frictional behavior of the coating and the workpiece material under process conditions in cutting. Based on the design of a custom pin-on disk test setup in a vertical turning machine build for elevated temperatures and sliding velocity for matching the conditions in machining, a friction model is determined for a TiN/AlTiN coated cutting tool. The non-linear friction behavior is then determined via a regression approach by training machine learning algorithms. A custom-made- python interface for the seamless incorporation of typical AI libraries and their models is presented for the software DEFORM 2D. The interface of the tool and the chip is discretized due to employed friction windows, for which the determined regression approach predicts the friction coefficient based on the calculated state variables of the FEA. Thus, this work presents a novel Grey-Box approach for locally predicting friction coefficients along the surface of coated cutting tools, which is the basis for an improved wear modelling of cutting tool coatings.

2:40pm **PP6-MoA-4 Coating-Dependant Thermomechanical Loading of Cutting Tools for Greybox Models**, *Thomas Bergs, Markus Meurer,* ***Mustapha Abouridouane [m.abouridouane@mti.rwth-aachen.de]***, Manufacturing Technology Institute (MTI) - RWTH Aachen University, Germany*; Kirsten Bobzin, Christian Kalscheuer, Muhammad Tayyab,* Surface Engineering Institute - RWTH Aachen University, Germany

For economically efficient cutting processes, cutting tool life can be extended through physical vapor deposition (PVD) coatings. However, imprecise tool life prediction models limit the cost-effective qualification of PVD coated tools. Analytical or simulation-based whitebox models mostly ignore coating effect on tool wear and cannot fully capture nonlinear interactions in cutting processes due to necessary simplifications of boundary conditions. In contrast, data-driven blackbox models can represent complex correlations but often lack an understanding of physical causality and robustness under variable conditions. To overcome these limitations, greybox models can be developed by coupling whitebox and blackbox models to create a balanced predictive framework. Such models require an inclusive dataset containing information on coating properties, realistic thermomechanical tool loading, process data and tool wear behavior. The current investigation focuses on determination of coating-dependent thermomechanical loading of cutting tools, required for development of greybox models. Monolayer TiAlCrSiN and bilayer TiAlCrSiN/TiAlCrSiON coatings were deposited on cemented carbide substrates and characterized. In order to assess thermomechanical tool loading, analogy tests representing orthogonal cutting were carried out on heat-treated C45 and 42CrMo4 steels. The process forces and tool temperatures were measured by dynamometer and high-speed infrared camera, respectively. Moreover, the heat flow into the tool was determined by placing a pyrometer directly under the rake face of the cutting inserts. The experimental data from coating properties and cutting tests contributed to the extension and validation of finite element chip formation simulation for coated tools. Thermomechanical stress distributions on coated tools with high spatial and temporal resolution were computed using the validated simulation model. The experimental as well as simulative data was combined to understand the effect of coating and workpiece material combinations on the process forces, tool temperatures as well as the resulting friction and tool wear behavior. The study contributes towards extension of existing numerical whitebox models for consideration of coating as well as determination of more accurate thermomechanical loading on PVD coated tools. The resulting high-resolution spatial and temporal thermomechanical tool loading data can be instrumental to the development of greybox models for tool life prediction.

3:00pm **PP6-MoA-5 Bridging the Gap Between Milling and Tribological Wear Mechanisms: Comparative Analysis of Coated Carbide Tools**, ***Amod Kashyap [amod.kashyap@kit.edu]***, Institute for Applied Materials (IAM-ZM), Micro-Tribology Centre (µTC), Karlsruhe Institute of Technology, Germany*; Amirmohammad Jamali,* Institute of Production Science (wbk), Karlsruhe Institute of Technology, Germany*; Johannes Schneider,* Institute for Applied Materials (IAM-ZM), Micro-Tribology Centre (µTC), Karlsruhe Institute of Technology, Germany*; Michael Stueber,* Institute for Applied Materials (IAM-AWP), Karlsruhe Institute of Technology, Germany*; Volker Schulze,* Institute of Production Science (wbk), Karlsruhe Institute of Technology, Germany

Milling tools used in metal manufacturing face severe challenges such as complex wear scenarios, heat generation and dissipation, and vibration, which lead to reduced tool life, poor surface quality, and higher operational costs. To address these issues, advanced coatings are applied to enhance their performance and longevity by reducing wear and friction, enabling higher cutting speeds and improved efficiency, and minimizing the formation of built-up edges. Coatings based on Titanium Nitride (TiN) and Aluminum Titanium Nitride (AlTiN) provide excellent heat resistance and hardness, crucial for maintaining tool integrity under high-temperature conditions.

The wear mechanisms of a milling tool vary depending on cutting parameters, and extensive research has been conducted on tool wear in coated milling tools with large-scale milling machines. Traditionally, researchers have attempted to evaluate coating performance using laboratory-based tribological setups. However, tribological tests do not accurately replicate the actual milling process. In this study, the authors aim to correlate tool wear in milling machines with wear observed in tribological model experiments. Milling tests were conducted with coated cemented carbide tools on C45 steel, and tribological tests involved coated cemented carbide cylinders against C45 discs. In-house TiN and AlTiN model coatings, deposited by pulsed-DC and high-power impulse magnetron sputtering techniques, were applied in these experiments. Tribological test parameters were optimized to replicate similar wear mechanisms on both the milling tools and coated cylinders, allowing for a detailed study of wear development through tribological testing only. Scanning electron and focussed ion beam microscopy including energy dispersive X-ray analysis were employed to analyse oxidation, adhesion, and diffusion wear on the coated carbide tools and cylinders. Additionally, the in-house-developed coatings were also compared with industrial coatings, enabling a comprehensive examination of wear mechanisms across different coatings.

3:20pm **PP6-MoA-6 Prediction of Tool Wear Depending on the Coating Architecture for Coated Cemented Carbide Tools by Machine Learning***,* *Benjamin Bergmann,* Institute of Production Engineering and Machine Tools - Leibniz University Hannover, Germany*; Christian Kalscheuer,* Surface Engineering Institute - RWTH Aachen University, Germany*; Berend Denkena,* Institute of Production Engineering and Machine Tools - Leibniz University Hannover, Germany*; Kirsten Bobzin, Xiaoyang Liu,* Surface Engineering Institute - RWTH Aachen University, Germany*;* ***Nico Junge [junge@ifw.uni-hannover.de],*** Institute of Production Engineering and Machine Tools - Leibniz University Hannover, Germany

Cutting tools based on cemented carbide are usually coated by physical vapor deposition. In machining operations, the specific characteristics of the process parameters and the machined material determine the different wear behavior. However, the utilization of diverse coating properties enables the targeted enhancement of wear resistance. Furthermore, the coatings are adjusted to the individual substrate. It could be shown, that the interaction between the substrate and the interlayer thickness and coating architecture exhibit a significant influence on the tool wear behavior. Due to the high complexity for predicting the influence of the interlayer on the wear behavior wear models are not available. Therefore, machine learning was used to predict the tool wear based on coating properties, considering the complex interaction between process parameters, tool and material.

In this study PVD coated cutting tools with three different interlayer thicknesses were prepared. This method is used to analyze different substrate-coating systems while preserving the properties of the functional layer of the tool. The initial coating properties such as residual stress, hardness and thermal conductivity were measured and served as input parameters for the ML- model. Afterward experimental wear investigations in turning different steels and process parameters were conducted. The wear data and the process parameters were also used as the input for the machine learning model. Different machine learning models such as support vector regression (SVR) and multilayer perceptron (MLP) were tested regarding the wear prediction. It can be shown, that the used models can predict the wear form and the size of wear for the turning operation depending on the operating time and the different coating properties, such as the interlayer thickness.

4:00pm **PP6-MoA-8 Greybox Modeling the Run-in and Wear Behavior of Milling Tools Coated with Arc-Evaporated TiAlN Based on Operando, in Situ and Ex Situ Analyses***,* ***Wolfgang Tillmann [wolfgang.tillmann@udo.edu],*** *Finn Rümenapf, Nelson FIlipe Lopes Dias, Simon Jaquet, Rafael Garcia Carballo, Dirk Biermann, Nils Denkmann, Jörg Debus,* TU Dortmund University, Germany **INVITED**

In modern machine manufacturing, a controlled cutting process is crucial for high workpiece quality and production efficiency. The dynamic stability of milling processes depends, e.g., on the cutting parameter values and the system behavior of the machine tool including the cutting tool. Milling tools are subjected to significantly more wear during dynamically unstable processes. To enhance wear resistance, cathodic arc evaporated TiAlN thin films are widely used. Throughout the cutting process, varying tribological loads alter the transient system behavior of the coated tools, which in turn impacts run-in behavior, tool wear, and lifetime. In this regard, the system behavior under varying dynamic load profiles remains largely unknown during the cutting process, thus complicating efforts to predict dynamic stability and tool wear accurately.

These challenges are addressed by using a greybox model approach designed to characterize the transient system behavior of TiAlN-coated tools. In a greybox model, experimental data of the steady-state and transient system behavior are exploited to reveal the wear initiation and development with respect to the dynamic run-in behavior. The experiments focus on the milling process of normalized C45 steel, utilizing tools coated with arc-evaporated TiAlN thin films. For the input of the greybox model a comprehensive dataset is produced, including *operando* cutting force measurements, *in situ* Raman spectroscopy, and *ex situ* analyses of chemical composition, hardness, and adhesion of the coatings pre- and post-cutting. A supervised machine learning model is used to enhance signal clarity and reliability of *in situ* input data. Furthermore, artificial neural networks with k-means clustering provide correlations between thin film properties, wear behavior and cutting performance. The combination of these AI-driven insights with physical and material-specific causalities allows the greybox model to predict tool wear progression and failure onset of the arc-evaporated TiAlN-coated milling tools.

Initial greybox model approaches demonstrate that the run-in behavior of the coated tools is influenced by the initial droplet distribution of the TiAlN, which in turn is affected by the choice of target material. This underlines the importance of considering the entire process, from coating deposition to tool performance. Additionally, a preliminary clustering of measurement data reveals meaningful patterns related to wear and stability. These first results highlight the potential of greybox models in describing the transient system behavior and predicting the lifetime of TiAlN-coated tools.

4:40pm **PP6-MoA-10 Determination of Residual Stress and Crystallite Size for TiAIN-Coated Milling Tools Using Laser-Spectroscopy-Based Grey-Box Modeling***,* ***Nils Denkmann [nils.denkmann@tu-dortmund.de],*** Department of Physics, TU Dortmund University, 44227 Dortmund, Germany*; Nelson Filipe Lopes Dias, Finn Rümenapf,* Institute of Materials Engineering, TU Dortmund University, 44227 Dortmund, Germany*; Simon Jaquet, Rafael Garcia Carballo, Dirk Biermann,* Institute of Machining Technology, TU Dortmund University, 44227 Dortmund, Germany*; Wolfgang Tillmann,* Institute of Materials Engineering, TU Dortmund University, 44227 Dortmund, Germany*; Jörg Debus,* Department of Physics, TU Dortmund University, 44227 Dortmund, Germany

TiAlN thin films are widely used in machining processes due to their high hardness and high wear resistance. However, continuous and intermittent thermo-mechanical loads during machining impair the structural properties of the thin film, e.g., the phase composition and the residual stress state. Such an impact alters the wear resistance of the thin film as well as the constitution of the tools, which ultimately leads to a drastic increase in tool wear. For a comprehensive understanding of the wear of coated milling tools, it is crucial to gain insight into the microscopic structural-chemical properties that determine early-predictively the degradation of the coating.

We use laser scattering spectroscopy combined with AI supported data analysis to determine changes in the residual stress and crystallite size of TiAlN coatings applied to milling tools for C45 steel machining. By utilizing confocal Raman scattering with micrometer spatial resolution, we measure the longitudinal and transversal optical and acoustic lattice vibrations, whose spectral line features grant access to the residual stress and crystallite size of TiAlN.

The *k*-means clustered changes in the residual stress and crystallite size h of TiAlN are correlated for initial and different material removal volumes of the TiAlN-coated tool. In the initial state and after minor material removal, the residual stress changes are given by (1.2 ± 0.6) GPa, while h fluctuates around 50 nm. In case of high material removal, the residual stress switches from compressive to positive tensile stress ranges with decreasing h. The sign switching in the residual stress is attributed to a temperature-induced spinodal segregation in fcc-TiN and fcc-AlN. This phase transformation appears to be present at h below about 30 nm. As the wear is significantly lower than for the uncoated reference tool, it can be assumed that the spinodal segregation has a wear-reducing effect.

In addition to that, a possible wear initiation for the TiAlN thin films is determined by the frequency of missing TiAlN Raman scattering signals at local tool surface positions. The *k*-means cluster analysis of the scattering spectra shows that with increasing material removal volume a non-specific background is formed in 5 % and 11 % of the cases, respectively.

Raman spectroscopy combined with grey-box modeling reveals possible wear initiations for the TiAlN thin films and outlines that the observed wear mitigation is related to the formation of self-organized nanostructures, so that structural-chemical changes at the tool surface may be used to develop robust and early-predictive criteria for wear.

5:00pm **PP6-MoA-11 Predicting Solid Particle Erosion of Metals: A Machine Learning Approach**,
***Stephen Brown* [stephen.brown@polymtl.ca]**, *Foutse Khomh,* Polytechnique Montréal, Canada*; Juan Manuel Mendez,* MDS Coating Technologies, Canada*; Marjorie Cavarroc,* Safran Tech, France*; Ludvik Martinu, Jolanta Ewa Klemberg-Sapieha,* Polytechnique Montréal, Canada

Solid particle erosion (SPE) is a tribological phenomenon in which a surface is impacted by a stream of particles, causing a gradual removal of the material. It is a critical challenge in aerospace, where compressor blades and other components are exposed to harsh particle-laden environments. Despite decades of research, accurately predicting SPE under diverse conditions remains difficult due to the non-linear relationships between erosion rates, material properties, and environmental factors. While several white-box models exist for the prediction of erosion, they rely on the use of empirically determined values that are sensitive to changes in erosion conditions and material properties, and are not easily adaptable to different erosion environments.

Machine learning (ML) offers a powerful alternative for handling variability and extracting insights from diverse datasets. This study compiles a database of over 1,000 erosion tests on metals based on the erosion literature and internal experiments, encompassing material and particle properties, experimental conditions, and article metadata. Using ML models such as XGBoost, Neural Networks, and Random Forests, erosion rates were predicted, achieving mean absolute errors (MAE) of 15-16% for the unseen test data. Model performance was further validated against interlaboratory test results from the ASTM G76 standard, with accurate predictions being made in two of three cases. The influence of different variables on erosion predictions was analyzed using feature importance metrics and partial dependence plots. Key features like particle velocity and impact angle showed expected effects, while the importance of target features such as density and Poisson's ratio was sometimes overstated due to their ability to act as classifiers for outlier materials.

These results demonstrate the potential of data-driven approaches to improve wear modeling by quantitatively predicting erosion rates across a wide range of conditions, while also highlighting the challenges arising from issues such as data sparsity and feature correlation.

5:20pm **PP6-MoA-12 Characterization of AlCrVY(O)N Thin Film Properties and Thermo-Mechanical Load Profiles in Machining AISI 304 Stainless Steel Using Greybox Modelling Approaches**,
***Erik Krumme* [erik.krumme@tu-dortmund.de]**, Institute of Machining Technology (ISF), TU Dortmund University, Germany*; Finn Rümenapf,* Chair of Materials Technology (LWT), TU Dortmund University, Germany*; Kai Donnerbauer,* Chair of Materials Test Engineering (WPT), TU Dortmund University, Germany*; Jannis Saelzer,* Institute of Machining Technology (ISF), TU Dortmund University, Germany*; Nelson Filipe Lopes Dias,* Chair of Materials Technology (LWT), TU Dortmund University, Germany*; Pascal Volke, Andreas Zabel,* Institute of Machining Technology (ISF), TU Dortmund University, Germany*; Wolfgang Tillmann,* Chair of Materials Technology (LWT), TU Dortmund University, Germany*; Frank Walther,* Chair of Materials Test Engineering (WPT), TU Dortmund University, Germany

The thermo-mechanical load collective prevailing in machining significantly determines the wear of coated carbide tools and therefore also has an influence on the productivity and sustainability of many industrial value chains. The tool wear can be described and predicted by developing greybox models, whereby it is known that the temperatures occurring in the chip formation zone have a greater impact on wear than the mechanical tool loads. AlCrVY(O)N thin films thus show significant promise for reducing tool wear due to lower friction and enhanced thermal stability at elevated temperatures compared to conventional thin films. Based on the complex coupling of friction, temperature and wear, the need for further development of such systems is substantial. To initiate greybox modeling of wear behavior, these thin-film systems were tested in whitebox approaches, i.e. when machining AISI 304 during an orthogonal turning process. As a benchmark, the thin films were compared to TiAlN and AlCrN thin films as well as uncoated cemented carbide tools. The thin film properties of AlCrVY(O)N on the cemented carbide inserts were evaluated and correlated with the cutting performance. The test set-up used, enables a comprehensive examination of the thermo-mechanical load collective concerning the measurement of the process forces and rake face temperatures. A variation of the cutting parameters was carried out to investigate the performance of the thin films under different levels of load. The tool wear identified was evaluated using blackbox approaches. In particular, a neural network for image segmentation was trained and applied to optical micrographs of the used tools. As a result, an automated evaluation of the tools was possible and new criteria for quantifying tool wear were developed. In order to improve the prediction of the transient tool wear behavior in form of cracks in the thin film and cutting edge failures, a further machine learning approach was chosen. For this purpose an autoencoder was developed and trained, which first analyzes the experimentally determined force measurement signals ex situ and can subsequently identify process windows of interest with regards to the tool wear behavior. The fundamental investigations show that the applied thin films on the inserts generally have a homogeneous chemical composition and a high hardness around 35 GPa. In the operational tests the temperatures on the rake face were reduced by using the AlCrVY(O)N thin films compared to TiAlN. Despite the low level of wear due to the short cutting time, image segmentation was validated as a suitable method for wear quantification.

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