Plasma and Vapor Deposition Processes
Room Town & Country A - Session PP1-2-MoA

PVD Coatings and Technologies II

Moderators: Christian Kalscheuer, IOT, RWTH Aachen, Germany, **Qi Yang**, National Research Council of Canada

2:00pm **PP1-2-MoA-2 Material-Dependent Loss in Deposition Rate of High Power Impulse Magnetron Sputtering Discharges***, **Martin Rudolph [martin.rudolph@iom-leipzig.de]**,* Leibniz Inst. of Surface Eng. (IOM), Germany*; Kateryna Barynova,* University of Iceland*; Nils Brenning,* KTH Stockholm, Sweden*; Swetha S. Babu,* University of Iceland*; Joel Fischer, Daniel Lundin,* Linköping University, Sweden*; Michael A. Raadu,* KTH Stockholm, Sweden*; Jon Tomas Gudmundsson,* University of Iceland, Sweden

High power impulse magnetron sputtering is an ionized physical vapor deposition technique in which the sputtered metal flux from the target is partially ionized. This enhances film properties like density and adhesion. At the same time, some of the produced metal ions are back-attracted to the target and therefore lost from the deposition process. We show that this loss in deposition rate is largely dependent on the sputter yield of the target material. Here, two extremes can be distinguished: 1) Discharges with low sputter yield targets are dominated by argon, and 2) discharges with high sputter yield targets are metal-rich. In the first case, the electron temperature must be significantly higher to enable sufficient ionization of predominantly the working gas to generate the experimentally observed high discharge currents. In those discharges we find strong electron energization by Ohmic heating in the ionization region extending beyond the cathode sheath. In the second case, we find that Ohmic heating is considerably weaker compared to the low sputter yield discharges. At the same time, frequent collisions with metal atom cool the electron population, which leads to a decrease in electron temperature. By examining a range of different target materials using the Ionization Region Model (IRM) we find a consistent trend of decreasing back-attraction probability and electron temperature as the sputter yield of the target material increases. A lower electron temperature increases the mean free path of ionization of sputtered species, shifting the average location of ionization away from the target. The much weaker electric fields at those locations compared to the target vicinity, ultimately facilitates ion escape toward the substrate, which thus explains the observed reduction in back-attraction.

2:20pm **PP1-2-MoA-3 Effect of Acetylene Gas Flow Rates on Target Poisoning, Phase Composition, Microstructure, Mechanical Properties and Corrosion Resistance of AlCrNbSiTiC High Entropy Alloy Carbide Thin Films***, Hsiang Yu Tsai, Yung Chin Yang,* National Taipei University of Technology, Taiwan*; Chia Lin Li,* Ming Chi University of Technology, Taiwan*; Bih Show Lou,* Chang Gung University, Taiwan*; **Jyh Wei Lee [jefflee@mail.mcut.edu.tw]**,* Ming Chi University of Technology, Taiwan

High entropy alloy carbide (HEAC) differs from conventional carbides, which are typically composed of one or two metallic elements. HEAC demonstrates remarkable properties, including an extremely high melting point, enhanced hardness, and superior wear resistance. In this study, AlCrNbSiTiCx HEAC thin films with varying carbon contents were deposited using a superimposed high power impulse magnetron sputtering (HiPIMS) and medium-frequency (MF) sputtering technique by a plasma emission monitoring (PEM) feedback control system. The optical emission signal of Cr element was monitored under different argon/acetylene gas flow ratios and the target poisoning effect was studied by the PEM system. The cross-sectional morphology, chemical composiitons, and crystal structure of the films were characterized using field emission scanning electron microscopy (FE-SEM), FE-electron probe microanalyzer (FE-EPMA), and X-ray diffraction (XRD), respectively. The mechanical properties of the HEAC thin films, including hardness, elastic modulus, adhesion, and wear resistance, were evaluated using nanoindentation, scratch testing, and pin-on-disk wear testing. The corrosion resistance of HEAC films in the in 0.5M sulfuric acid aqueous solution was explored. This study systematically investigated the influence of target poisoning ratios and carbon content on the phase composition, microstructure, mechanical properties, and corrosion resistance of AlCrNbSiTiCx HEAC thin films. Potential applications of these HEACS films were also proposed in this work.

2:40pm **PP1-2-MoA-4 Duplex Coating Process by Plasma Enhanced Magnetron Sputtering***, **Jianliang Lin [jlin@swri.org]**,* Southwest Research Institute, USA

Metallic substrates can be treated by a combination of nitriding and subsequent deposition of a physical vapor deposition (PVD) coating to improve coating adhesion, wear/abrasion resistance, and corrosion resistance. The combination of the two processes is known as duplex treatment. In general, conventional nitriding treatment and PVD coating deposition are typically performed as two separate processes in distinct facilities and environments. Consequently, the lead time and production cost are not optimized. We present a duplex coating process by integrating plasma nitriding and magnetron sputtering using hot filament assisted and plasma enhanced magnetron sputtering (PEMS) within the same facility. In the process, a global nitrogen plasma is generated by impact ionization from electrons emitted from the hot filaments and attracted towards the substrate surface for nitriding. In this study, the effects of the PEMS process on the structure and properties of the nitrided stainless steel have been studied. The PEMS treated stainless steel exhibited greatly improved surface hardness, wear resistance, and hydrophobicity in oil formula. In addition, duplex TiSiCN and DLC coatings deposited using the integrated process showed improved mechanical properties and adhesion as compared to the coatings deposited without the duplex treatment.

4:40pm **PP1-2-MoA-10 Determination of Mechanical Properties of PVD Tool Coatings Using Machine Learning***, Kirsten Bobzin, Christian Kalscheuer, **Xiaoyang Liu [liu@iot.rwth-aachen.de]**,* Surface Engineering Institute - RWTH Aachen University, Germany

The wear resistance of physical vapor deposition (PVD) coatings is heavily influenced by their elastic and plastic properties. These properties serve as essential inputs for finite element method (FEM) simulations to predict tool wear, including the elastic modulus for the characterization of elastic properties and parameters of the Johnson-Cook model for the description of the plastic behavior. A precise determination of these parameters is required for simulation of tool wear. In this study, machine learning models are developed to directly map load-depth curves from nanoindentations on TiAlSiN and TiAlCrN coatings to parameters of coatings in FEM. An FEM simulation model of nanoindentation is employed to generate a dataset comprising load-depth curves resulting from a wide range of input material properties. Several machine learning models including support vector regression (SVR), multilayer perceptron (MLP), long short-term memory (LSTM) and gated recurrent unit (GRU) are then trained, validated, and compared using this dataset. The input to these models consists of simulated load-depth curves, with the target being parameters required for the definition of the material in commercial FEM softwares. Among these machine learning models, GRU achieves the best prediction performance. Ultimately, GRU is used to predict material parameters of TiAlSiN and TiAlCrN coatings based on experimental load-depth curves. FEM simulations using the GRU-predicted material parameters show excellent alignment with experimental measurements, achieving accurate results in a single iteration without further parameter adjustments. The determined parameters can be directly used as reasonable inputs for further FEM simulations as parts of a Greybox model to predict tool wear during cutting.

5:00pm **PP1-2-MoA-11 Experimental and Simulative Investigation of Crack Growth in TiAlCrN PVD Coatings***, **Ujjwal Suri [u.suri@iwm.rwth-aachen.de]**, Felix Weber, Christoph Broeckmann,* Institute of Applied Powder Metallurgy and Ceramics (IAPK) at RWTH Aachen e.V., Germany*; Kirsten Bobzin, Christian Kalscheuer, Xiaoyang Liu,* RWTH Aachen University, Surface Engineering Institute (IOT), Germany

Hard physical vapor deposition (PVD) coatings are widely used as protective layers on cemented carbide tools due to their exceptional mechanical properties. However, these coatings can be susceptible to damage and cracking. Gaining a deeper understanding of how the coating microstructure influences the cracking behavior is essential. Moreover, most tool wear prediction does not include the effect of the cracking behavior. Thus, crack initiation and propagation under external loads and its contribution to tool wear should be investigated. A precise micromechanical simulation of cracks could enhance the accuracy of tool wear simulations in cutting applications.

This study combines experimental and mesoscale simulation to investigate the cracking behavior of a TiAlCrN PVD coated cemented carbide tool. Initially, nanoindentations coupled with inverse FEM simulations are conducted to determine mechanical properties of coatings, specifically Young's modulus and parameters for the Ludwik-Hollomon model. These properties are then applied to simulate high-load nanoindentation at a macroscopic scale. Subsequently, scanning electron microscopy (SEM) is applied to characterize the grain morphology. Using this data, a representative finite element model is developed. Numerical simulations of the local crack initiation and growth are performed based on the implemented model in combination with the extended finite element method (XFEM). SEM micrographs taken after indentation are analyzed to study crack behavior, enabling a correlation between experimental results and numerical simulations.

The combined experimental and detailed numerical modelling approach facilitates insights into how microstructural parameters including grain size and orientation influence crack growth in the coating system. This study presents a combined analysis using experimental nanoindentation and a mesoscopic simulation model of the nanoindentation to investigate the crack growth in PVD coated cemented carbide. The correlation of experimental and simulative results allows a detailed study of the interaction of microstructure and crack growth in PVD coatings. Models comparable to the one here presented may be used in future work for optimization of coated cemented carbide tools.

5:20pm **PP1-2-MoA-12 Characteristics of TiAlN+X Coatings for Inconel Machining using Advanced Arc Technology**, ***Ryosuke Takei [takei.ryosuke@kobelco.com]**, Shinichi Tanifuji, S. Hirota,* Kobe Steel Ltd., Japan; *M. Tona, N. Hirata,* Ayabo, Ltd., Japan

Inconel is a material with low thermal conductivity, making it challenging to machine due to the high cutting edge temperature and rapid tool wear. To extend tool life, coating performance is crucial. Although various coatings have been developed for machining Inconel, an optimal solution has yet to be established.

Common coating processes for cutting tools include cathodic vacuum arc (CVA), sputtering, and chemical vapor deposition (CVD), each with its limitations. Sputtering produces smooth coatings but suffers from lower hardness and productivity. CVD coatings offer excellent toughness at high temperatures, making them suitable for turning; however, their intrinsic tensile stress makes them less ideal for milling. The arc process enables dense coatings with high compressive stress and high productivity, but excessive droplet deposition increases surface roughness, reducing cutting performance. In Inconel machining, it has been reported that work material can fill voids around droplets, leading to film damage.

A previous study by KOBELCO investigated AlCrN coatings using both a conventional arc evaporation source and a novel "μ-ARC" source. The μ-ARC process was found to reduce surface roughness and micro-particles (MPs), improving durability in cutting tests. However, due to the chemical reactivity between AlCrN and nickel-based materials, Cr-containing coatings are generally unsuitable for Inconel machining, and TiAlN or TiAlN+X coatings are commonly used instead.

This study explores the deposition of TiAlN and TiAlN+X films using both conventional and μ-ARC evaporation sources. The effects of the evaporation source and metal X addition on the film's microstructure, mechanical properties, and crystal structure are analyzed. Based on these evaluations, optimal deposition conditions for carbide end mills were determined, and machining performance of TiAlN and TiAlN+X coated tools in Inconel cutting was evaluated. The findings provide insights into the development of high-performance coatings with improved durability and cutting efficiency.

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