Plasma and Vapor Deposition Processes
Room Town & Country A - Session PP1-1-MoM

PVD Coatings and Technologies I

Moderator: Christian Kalscheuer, IOT, RWTH Aachen, Germany

10:00am **PP1-1-MoM-1 Optimizing Sputter-Deposited MoS2 Coatings: Insights from Monte Carlo Simulations and In-Situ Plasma Diagnostics***, **Alexander Mings [ajmings@sandia.gov]**, Steven Larson, Kyle Doorman, Tomas Babuska, John Curry, Remi Dingreville, David Adams,* Sandia National Laboratories, USA

Sputter-deposited molybdenum disulfide (MoS_2) coatings are widely utilized in aerospace applications, primarily due to their exceptional reliability and ultralow friction in vacuum environments. However, the unique structure of MoS_2 often leads to high porosity in sputtered coatings which can significantly compromise wear life and accelerate film oxidation. To address these challenges, engineers typically engage in costly process development, varying deposition parameters to maximize film density with limited available heuristics. This process development is also equipment specific and must be repeated when a process needs to be transferred.

This study explores how the kinetic energy of species impacting the substrate during the growth of MoS_2 films influences their porosity. We employ Monte Carlo simulations using both SRIM (Stopping and Range of Ions in Matter) and SIMTRA (Simulating the Transport of Atoms from the Source to the Substrate) to analyze the contributions of both sputtered atoms and backscattered neutrals. By correlating these findings with nanoindentation hardness, we gain insights into how deposition dynamics affect coating porosity. Additionally, we compare the simulation results to in-situ measurements made with a Retarding Field Energy Analyzer (RFEA) positioned at the substrate. Our findings reveal the energy flux necessary to produce dense coatings, which can be used in combination with a RFEA to provide essential feedback for process development. This approach has the potential to both greatly accelerate process transfer and enhance the film performance of existing MoS_2 processes.

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10:20am **PP1-1-MoM-2 HiPIMS and Digitalization: Increasing Efficiency in Machining***, **Stephan Bolz [stephan.bolz@cemecon.de]**, Biljana Mesic, Oliver Lemmer, Christoph Feig,* CemeCon AG, Germany

The presentation "HiPIMS and Digitalization: Increasing Efficiency in Machining" shows how modern digitalization and innovative coating technologies accelerate the development of HiPIMS coatings for cutting tools.

The focus is on using a HiPIMS coating system “CC800 HiPIMS,” for which a digital twin model exists that captures and analyzes large amounts of data.

Machine data are first collected via an OPC-UA interface, persisted in a database, and then transferred into the digital twin. This allows simulation results to be quickly integrated into process development. Consequently, only a few validation experiments are needed, saving time and resources. The simulation-optimized HiPIMS process parameters enable the deposition of coatings that are denser and harder than ever before. These were tested on cutting tools and achieved better results than previous layers.

Overall, the talk demonstrates how the combination of HiPIMS technology and digitalization increases efficiency in coating development, improves product quality, and strengthens competitiveness in high-performance machining.

10:40am **PP1-1-MoM-3 From Poisoned Targets to Healthy Models: The Quest for Parameters***, **Diederik Depla [Diederik.Depla@ugent.be]**,* Ghent University, Belgium **INVITED**

The conceptual simplicity of reactive magnetron sputtering facilitates the description of global trends in process curves characteristic of reactive magnetron sputtering. However, achieving a quantitative description of these trends through simulations remains far more challenging, as the critical bottleneck of every modelling effort lies in the determination of accurate input parameters. Following a brief introduction to the RSD model, this paper provides an overview of several experimental methodologies designed to extract the parameters essential for its implementation. A central parameter in any thin-film deposition technique is the deposition rate. While its determination in metallic mode is relatively straightforward, the task becomes substantially more complex in poisoned mode due to the limited availability of sputter yield data for oxides. Our experiments reveal that in poisoned mode sputter yields exhibit a pronounced dependence on process conditions. Monte Carlo simulations, moreover, uncover a remarkable material-independent correlation between reported partial yields for oxides and experimentally measured yields in poisoned mode. Another crucial quantity, the ion-induced electron yield, can only be reliably determined experimentally, even for metals. By employing empirical scaling laws, however, it becomes feasible to estimate these yields under poisoned-mode conditions. The strong influence of chemisorption on the electron yield explains the discharge voltage behaviour in metallic mode. The influence of chemisorption on target poisoning emerges as the next major challenge, particularly as a novel strategy to control the reactive sputtering process exposes discrepancies between the current formulation of the model and experimental observations. Nevertheless, this measuring strategy provides compelling evidence that the RSD model’s prediction of double hysteresis behaviour is fundamentally correct.

11:20am **PP1-1-MoM-5 Advanced YSZ Coatings Deposited by Magnetron Sputtering for High-Temperature Applications***, **Imene Toumi [imene.toumi@utt.fr]**,* Université de Technologie de Troyes, France*; Sofiane Achache,* Université de technologie de Troyes, France*; Akram Alhussein, Benoit Panicaud,* Université de Technologie de Troyes, France

Thermal barrier coatings (TBCs) are essential for extending the lifetime and efficiency of components exposed to extreme thermal environments, particularly in aerospace and energy systems [1-2]. Yttria-stabilized zirconia (YSZ) remains the benchmark topcoat material due to its low thermal conductivity, high fracture toughness, and outstanding thermal stability [1-4]. The performance of these coatings is strongly governed by the stabilization of the metastable tetragonal phase, which depends on both yttria content and deposition conditions [5].

In this study, YSZ thin films were deposited by dual-target reactive magnetron sputtering (Zr + Y) under an Ar/O_2 atmosphere. A parametric analysis was conducted to evaluate the effects of oxygen flow rate, substrate position, scanning amplitude, and yttrium doping level (expressed as Y_2O_3 content) on film growth, chemical composition, and crystalline structure.

Physicochemical and mechanical characterizations were performed using X-ray diffraction (XRD), energy-dispersive spectroscopy (EDS), scanning electron microscopy (SEM), and nanoindentation. The optimal yttria content (Y_2O_3) was found to be ≈ 2.9 mol%, ensuring stable tetragonal phase formation.

Furthermore, the thermal stability of the prepared coatings was assessed through annealing cycles at 500 °C, 750 °C, and 1200 °C. The study aims to evaluate the stability of the tetragonal phase at elevated temperatures and to investigate the microstructural evolution of YSZ thin films.

This work establishes a multi-parameter optimization strategy for YSZ thin films, contributing to the design of next-generation TBCs with improved structural integrity and reliability in harsh service conditions.

11:40am **PP1-1-MoM-6 Low-Temperature Synthesis of Ti_2AC (A = Si or Ge) Max-Based Coatings via Highly Ionized Growth Techniques***, Arno Gitschthaler, Philipp Dörflinger, Rainer Hahn,* Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria*; Jürgen Ramm, Klaus Böbel,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials GmbH, Germany*; Eleni Ntemou, Daniel Primetzhofer,* Department of Physics and Astronomy, Uppsala University, Sweden*; Dominik Fuchs, Andreas Limbeck,* Institute of Chemical Technologies and Analytics, TU Wien, Austria*; Peter Švec,* Institute of Physics, Slovak Academy of Sciences, Slovakia*; Anton Davydok, Christina Krywka,* Institute of Materials Physics, Helmholtz Zentrum Hereon, Germany*; **Helmut Riedl [helmut.riedl@tuwien.ac.at]**,* Institute of Materials Science and Technology, TU Wien, Austria

MAX phases are a unique class of nanolaminated compounds that combine metallic and ceramic properties, offering excellent electrical and thermal conductivity together with remarkable resistance to creep, oxidation, and corrosion. These characteristics make them highly attractive as protective and functional coatings for next-generation hydrogen technologies. However, conventional sputtering techniques struggle to provide suitable growth conditions at reduced synthesis temperatures, often leading to phase instability and the formation of competing phases. Despite more than two decades of research on Ti–A–C (A = Si or Ge) MAX coatings [1,2], it has yet to be achieved to deposit them under less harsh, more practical conditions. To address this issue, Ti_2-A-C (A = Si or Ge) thin films were deposited by cathodic arc evaporation (CAE) and high-power impulse magnetron sputtering (HiPIMS) of metallic TiA (A = Si or Ge) targets in reactive Ar/C_2H_2 plasma atmospheres. To understand the relationship between deposition parameters, chemical composition, and phase formation, the resulting films were comprehensively characterized using high-resolution techniques, including ToF-ERDA-calibrated GD-OES, 2D-BBXRD, and t-CSXRD measurements. Subsequently, these results are correlated with application near electrochemical tests. Overall, these analyses demonstrate, for the first time, that Ti_2-A-C MAX-based coatings can be successfully synthesized by reactive CAE and HIPIMS at temperatures as low as 550 °C and rise their potential for use cases in hydrogen technologies.

[1] Emmerlich J, Palmquist J-P, Högberg H, Molina-Aldareguia JM, Hultman L. Growth of Ti3SiC2 Thin Films by Elemental Target Magnetron Sputtering. J Appl Phys. 2004;96: 4817. doi:10.1063/1.1790571

[2] Högberg H, Eklund P, Emmerlich J, Birch J, Hultman L. Epitaxial Ti2GeC, Ti3GeC2, and Ti4GeC3 MAX-phase thin films grown by magnetron sputtering. J Mater Res. 2005;20: 779–782. doi:10.1557/JMR.2005.0105

12:00pm **PP1-1-MoM-7 Development of a Thickness Ratio Design Model for TiN/Ti/TiN/Ti Coating: Stress and Energy Relief Analysis***,* ***Yi-Cheng Yang [richardyang329@gmail.com],*** Department of Engineering and System Science National Tsing Hua University, Taiwan

Transition metal nitride (TMeN) coatings deposited by physical vapor deposition (PVD) are often subjected to high residual stress, which may induce delamination and failure of coatings. Introducing a metal interlayer between the coating and substrate is one of the common approach to relieve residual stress. However, the design of interlayer thickness in commercial applications generally lacks quantitative evaluation. In our previous studies, we developed an energy-balance model to quantitatively evaluate the stress and energy relief efficiency of coatings using ZrN/Ti, ZrN/Zr and TiN/Ti as model systems. With the growing demand for multilayer structures, optimizing the thickness ratio between coating and the metal interlayer for effective stress and energy relief has become essential for improving coating performance and process efficiency. Therefore, this study aims to evaluate the thickness ratio between coating and interlayer using TiN/Ti/TiN/Ti as a model system. By employing the energy-balance model under bilayer conditions, the effect of varying Ti and TiN layer thickness ratios on stress and energy relief behavior will be comprehensively analyzed. In this study, TiN coatings were deposited on Si substrates using DC unbalanced magnetron sputtering (DC-UBMS). Residual stress was measured by laser curvature measurement and the average X-ray strain (AXS) method. Based on the optimized model, the influence of thickness ratio on the stress and energy relief in multi-layer structures can be quantitatively evaluated.

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