Plasma and Vapor Deposition Processes
Room Town & Country B - Session PP7-FrM

Modeling and Data-Driven Methods for Process Design, Analysis and Control

Moderator: Petr Zikán, PlasmaSolve s.r.o., Czechia

10:20am **PP7-FrM-8 Insights on Plasma Processing from Multi-Scale Physical and Data-Driven Modeling**, *L. Vialetto,* Stanford University, USA*; T. Gergs,* Kiel University, Germany*; I. Chaerony Siffa,* Leibniz Institute for Plasma Science and Technology (INP), Germany*; C. Stüwe,* Kiel University, Germany*; T. Mussenbrock,* Ruhr University Bochum, Germany*; M. Becker,* Leibniz Institute for Plasma Science and Technology (INP), Germany*; **Jan Trieschmann (jt@tf.uni-kiel.de)**,* Kiel University, Germany **INVITED**

The theoretical description of plasma processing provides a formidable task that has been addressed by analytical modeling and numerical simulation for decades. Although the continuous increase in compute power has enabled simulation studies of the gas discharge physics in great detail, many open questions remain. This is reasoned by the extremely complex dynamics of multi-component plasmas facing solid surfaces, involving a large number of processes in the plasma and in the solid, as well as their plasma-surface interaction. The time and length scales of these physico-chemical processes span many orders of magnitude. Well separated scales often allow for the description of a given phenomenon on its respective scales, paired with a hierarchical coupling. This coupling is often rather static and realized via oversimplifying assumptions (e.g., tabulated coefficients), and may be biased-by-experience. Advantage can be taken from more unbiased data-driven approaches, which are derived from high fidelity data obtained from physical models at the lower scales. Moreover, the description of certain physical mechanisms may be substituted by data-driven sub-models (e.g., electric field calculation or transport parameters from a kinetic description). Correspondingly, a hierarchy of physical and data-driven models may be derived, linking global process quantities (e.g., pressure, voltage, current) to microscopic process quantities (e.g., thin film composition, electrical properties).

This approach is exemplified by the investigation of a low-pressure partially-magnetized capacitively coupled radio frequency discharge for the sputter deposition of silicon oxide thin films. The model is implemented in the OpenFOAM framework, extended by a Particle In Cell/Monte Carlo Collisions (PIC/MCC) implementation and coupled to a system of fluid equations for the neutral background. The surface evolution is described by a system of rate equations, which takes into account physical sputtering, chemisorption, physisorption, and surface diffusion of adatoms. The dynamics of physical sputtering are included using an artificial neural network model trained on surface kinetics data with varying stoichiometry from Monte Carlo simulations. It is argued that the versatility of the implementation also allows to use this model in a broader range of applications, such as plasma etching.

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11:00am **PP7-FrM-10 Utilizing Digital Twin Technology for Automated Coating Recipe Development**, ***Petr Zikan (zikan@plasmasolve.com)**, A. Obrusnik,* PlasmaSolve s.r.o., Czechia

Recent developments in the field of coating technology have seen a rise in the adoption of process modeling and digital twin tools. The primary motivation for this shift is the extended duration and unpredictability of process transfers and scaling in coating applications. Moreover, these technologies are now beginning to contribute to energy reduction in coating processes.

In our previous work, we introduced a Digital Twin model for coaters, integrated into the MatSight framework by PlasmaSolve. This model demonstrated high accuracy in predicting the composition and key performance characteristics (such as hardness and residual stress) of coatings, utilizing a dataset of only eight characterized samples for training. This achievement was made possible by a hybrid process model that merges simulations of physical processes and chemistry with machine learning techniques. By incorporating knowledge of the coater's physical limitations, the model significantly reduced the need for extensive training experiments.

This contribution advances our research by tackling an inverse problem: using the Digital Twin model to create a coating recipe based on defined material specifications. These specifications include the number of layers, the thickness and composition of each layer, and the target hardness/residual stress for the complete stack. The model generates a recipe file compatible with coater operations, allowing for immediate implementation and validation of model predictions.

Furthermore, we illustrate how the Digital Twin model can be seamlessly integrated with other PVD simulation tools, offering a comprehensive view of the coating process. A case in point is the integration with the MatSight Coating Uniformity App, which enhances understanding of the coating's thickness distribution and the variations in ion bombardment and composition across a 3D object.

11:20am **PP7-FrM-11 Open-Source Plasma Modelling for Thin-Film Technologies with the Simulation Tool PICLas**, ***Paul Nizenkov (nizenkov@boltzplatz.eu)**, A. Mirza, S. Copplestone, J. Beyer,* boltzplatz - numerical plasma dynamics GmbH, Germany

Simulating technical plasmas or highly rarefied gases in vacuum chambers presents a significant challenge due to the complexity of processes such as electron kinetics and strong non-equilibrium effects. To address these challenges, gas kinetic approaches are often employed. These approaches describe the medium not as a continuum, but as a stream of particles, including atoms, ions, and electrons.

This talk introduces PICLas, an open-source simulation tool originally developed for the simulation of space systems such as atmospheric re-entry & electric propulsion and now applied in various technical fields for simulating plasma processes. PICLas is based on gas kinetic approaches, utilizing particle methods like Particle in Cell (PIC) and Direct Simulation Monte Carlo (DSMC). A distinctive feature of PICLas is its modular structure, which allows the software to be used either as a pure DSMC or pure PIC solver. Combining these methods opens up exciting possibilities, such as simulating collisional plasmas.

The development of an intelligent graphical user interface aims to make this complex modeling more accessible to technical developers. This interface leverages modern web-based technologies and other open-source projects for cost-effective development. The talk will demonstrate how these technologies, combined with PICLas, can streamline the pre-processing, simulation setup, and post-processing in numerical simulation projects. Furthermore, the talk shall present different application examples, where the code has been tested and validated for thin-film technologies.

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