New Horizons in Coatings and Thin Films
Room Town & Country B - Session F5-MoM

Machine Learning and Process Modeling for Coating Design and Production

Moderators: Adam Obrusnik, PlasmaSolve s.r.o., Czechia, **Ferenc Tasnadi**, Linköping University, Sweden, **Petr Zikán**, PlasmaSolve s.r.o., Czechia

10:00am **F5-MoM-1 Thin Film Process Modeling at Different Scales - from Kinetic Simulation to Digital Twin*, Andreas Pflug,*** Fraunhofer Institute for Surface Engineering and Thin Films IST, Germany **INVITED**

Modern products require coating stacks with increased complexity and precision as well as improved throughput, reproducibility and environmental footprint. Simulation is a valuable asset to reach these goals by modelling deposition reactor dynamics as well as thin film growth on atomistic level.

The various physical scales of thin film deposition can be addressed by either model-driven or data-driven codes. The first category is based on physically accurate models, that need only few unknown internal parameters but require high computational power. Examples are the Direct Simulation Monte Carlo (DSMC) and Particle-in-Cell Monte-Carlo (PIC-MC) methods for description of gas flow and plasma processes at low pressure and Molecular Dynamics (MD) or kinetic Monte Carlo (kMC) methods for modeling atomistic processes in thin film growth. Despite of their high computational demand, these methods are useful for getting insights into the functionality of novel deposition setups and plasma sources.

A complementary approach uses data-driven simulation codes, which are based on simplified, semi-empirical models or machine learning methods. On the one hand, they need a significant amount of internal data in order to be adjusted to represent specific process conditions, on the other hand they usually require only low computational power, which enables to do parameter optimization or use them as real-time capable digital twins for model-based in-situ process control.

This talk shows various examples for model-based simulation of PVD processes. Furthermore, it demonstrates how to use data obtained by physical modeling in order to create a digital twin for prediction of the coating uniformity on 3D substrates in a sputter reactor for optical coatings.

10:40am **F5-MoM-3 Coater-Scale Model of DC Magnetron Sputtering*, Andrej Roštek,*** Masaryk University / PlasmaSolve s.r.o., Czechia*; P. Zikán,* PlasmaSolve s.r.o., Czechia*; J. Tungli,* Masaryk University, Czechia*; A. Obrusník,* PlasmaSolve s.r.o., Czechia

Magnetron sputtering is a widely used technique for the deposition of metal and compound layers for numerous technical applications. However, optimizing a sputtering process is a challenging task, especially since each industrial customer has specific requirements and expectations.

In order to improve properties of deposited coatings it is essential to understand the physics influencing them. Since the physical processes in magnetron sputtering are complex, it is often necessary to employ computer simulations. There has been a lot of work done in this regard [1-3], however, the simulations typically focused only on one part of a sputtering process, such as target erosion, sputtered atom transport, or the discharge properties.

This contribution attempts to provide a bigger picture by creating a coater-scale model which is a combination of two sub-models: (1) The bulk plasma model, which is a fluid model describing the plasma between the target and the substrate. It mostly affects ion bombardment. (2) The cathode plasma model, which is a particle-based model where ions and electrons are traced in the electric and magnetic field in the close vicinity of the target where the plasma sheath resides. This model affects mostly the target erosion. Its implementation is similar to our previous model from [4].

Together, these two models provide insight into various phenomena such as ion flux distribution, which determines target erosion, and the magnitude of ion bombardment at the substrates, which is a key determiner of the coating performance properties (residual stress, hardness, composition). Moreover, parametric studies can be performed so that the influence of pressure, substrate bias voltage, position of the electrodes, and others can be studied.

This model will be validated against experimental data.

References:

[1] C. Feist, A. Plankensteiner, J. Winkler *Studying Target Erosion in Planar Sputtering Magnetrons Using a Discrete Model for Energetic Electrons*Proceedings of the Conference: COMSOL, 2013

[2] S. Mahieu et al. *Monte Carlo simulation of the transport of atoms in DC magnetron sputtering* Nucl. Instrum. Methods Phys. Res. B, 243 (2), 2006, 313-319

[3] E. Shidoji, N. Nakano, T. Makabe *Numerical simulation of the discharge in d.c. magnetron sputtering* Thin Solid Films, 351 (1–2), 1999, 37-41

[4] A. Rostek *Simulating ion flux to 3D parts in vacuum arc coating: Investigating effect of part size using novel particle-based model* Surf. Coat. Technol., 449, 2022, 128954

11:00am **F5-MoM-4 High-Throughput Simulations to Predict History Dependence of Feedback Control During Reactive Magnetron Sputtering*, Josja Van Bever,*** *K. Strijckmans, D. Depla,* Ghent University, Belgium

Feedback process control [1] of reactive sputtering is often required to achieve specific thin film properties. Although conceptually simple, it is far from trivial to make it reliable and reproducible. Two major problems can be identified.

First, depending on the initial state of the process two S-shaped process curves can be obtained under certain conditions [1]. Many suggestions have been made for the observation of this "*double hysteresis phenomenon*" such as target erosion, chamber heating, or anode effects. But even when these effects are excluded, the phenomenon can still be observed (figure 1) [2]. Hence it seems to be of a fundamental nature. Independently of the experimental observations, the simulation of the processes at the cathode facing the gas discharge led to the prediction of a double hysteresis [3].

Secondly, the *convergence of the feedback process* strongly depends on the history of the target process. Simulation of the transient target states may therefore also assists to improve this convergence.

In the first part of the presentation we present *high-throughput simulations* for double hysteresis behavior as a function of different process and material parameters [4, 5]. *New measures* are introduced that characterize the hysteresis with a single number and that vary in a continuous way as a function of these parameters. This allows us to *elucidate the nature of the double valued state during feedback control* and to explain for which materials and under which conditions this behavior is expected to occur (figures 2 and 3) [4].

In the second part we discuss the *application of this analysis* to feedback measurements of aluminum. A correct preparation of the target subsurface can speed up the feedback process and a *first direct proof of double hysteresis during feedback control* is delivered. Next, the measures from the high-throughput simulations are applied to investigate the role of diffusion [6] on the double valued nature of the process conditions achieved during feedback control.

Additional figures and references are found in the supplementary material.

11:20am **F5-MoM-5 Evatec Fabric – a Thin-Film Process and -Metrology Data Tracking System for Large-Scale, Automated Data Analysis in R&D Labs*, Clemens Nyffeler,*** *O. Rattunde, D. Jaeger, H. Zangerle, R. Gmuender,* Evatec AG, Switzerland

Managing data in an R&D lab is often tedious manual work and leads to heterogenous, incomplete data. To ensure reproducibility, information about experimental setups, process hardware, and -conditions, and sample pre-treatment, must be kept in addition to the primary results. Consolidating and harmonizing datasets for large-scale, overarching data science projects constitutes a substantial additional effort.

At Evatec we developed a system, designed to automate these things in the specific context of thin film process development and verification. Substrate information, hardware configuration, process log-data, and measurement results are linked together based on wafer-ID.

In contrast to traditional manufacturing execution systems (MES), the *Evatec Fabric* can dynamically reconstruct the chronology of events for each wafer without need to define a process flow in advance. This allows our scientists and engineers a wide degree of flexibility in carrying out their work.

A data-processing component, programmed in python, uses various algorithms, models, and data-fitting techniques to process the raw data, produced by process systems and metrology instruments. It extracts useful parameters and statistics that are stored in a highly structured and contextualized way, enabling data science and machine learning projects based on clean, homogenous data.

11:40am **F5-MoM-6 Predicting Reactive PVD Processes Using Global Process Modeling – a Physics-Based Alternative to Machine Learning***, **Petr Zikán**, A. Obrusnik,* PlasmaSolve s.r.o., Czechia

Developing, transferring, or troubleshooting reactive PVD processes has always been a challenge. This can be partly attributed to the non-linear behavior of these processes. Additionally, the fundamental variables that drive the physics (e.g., plasma density and potential, the energy of sputtered and ionic species, …) are hard to measure, thus, often unknown in practice.

Another typical challenge is the number of consistent experiments available about the process. Experiments and their analysis are expensive and time-consuming. It is not uncommon that there are only a few (< 10) experiments available. This is the main limitation of machine-learning methods as these require large data sets (> 100).

In this contribution, we describe an alternative, physics-based approach that works well even with a low number of experiments. We illustrate that it is possible to formulate such a model for a whole coater that is either free of fitting parameters or contains only a few of them and they have a clear physical meaning. These models additionally contain coefficients, such as pumping speed, sputtering yields, or effective coating areas. These parameters are either known (pumping speed), can be obtained from the literature (sputtering yields), or can be pre-computed using 2D or 3D simulations (effective coating areas) for the coater and loading at hand.

Once created, such a model can reproduce the material composition across coaters and coater conditions with the accuracy of a few atomic percent. By correlating the process model outputs with literature data, the tool can also make predictions about the performance parameters of the coating (e.g., hardness). The approach will be illustrated in the case of nitride- or carbide-based ceramic coatings.

The specific global process model being discussed is not a simulation tool only but also an analytical tool in the sense that it works with a coater log at the input and combines machine log analytics with simulation data. As of submitting this abstract, the tool was already leveraged in five projects aimed either at process transfer between coaters (R&D scale) or achieving better process reproducibility (at MP-scale).

12:00pm **F5-MoM-7 Structure and Crystallographic Properties of Multi-Material Coatings Deposited in a Combinatorial Sputter Plant Compared to Simulations from the Machine Level to Microstructure***, **David Böhm**,* TU Wien, Austria*; T. Schrefl,* Danube University Krems, Austria*; A. Eder,* MIBA High Tech Coatings GmbH, Austria*; C. Eisenmenger-Sittner,* TU Wien, Austria

Structure and crystallographic properties of multi-material thin films can be described with an interactive ray tracing software that simulates film deposition in arbitrary sputtering geometries, the so-called Virtual Machine (VM). Although based on a line-of-sight model, the VM also takes into account the decay of the flux density of the particles due to gas phase scattering. To further enhance the prediction capabilities of the VM a microstructure simulation package, based on rate equations and on the Potts Modell, was built.

At the machine level the VM recreates a real combinatorial DC-sputter plant from 3D models including the static arrangement of multiple targets, the substrate and eventual obstacles, as well as dynamics like e. g. rotating substrate holders. For the deposition process, individual sample points can be defined on the substrate to which the line-of-sight model is applied, taking kinematics into account. The resulting thickness and sequence of the layers is used to visualize the thickness-resolved composition. Post-processing the time dependent thickness and temperature data the crystallographic phases with their associated XRD patterns are calculated from a library of binary phase diagrams for the simulated film.

Applying the rate-equation model to a generated layer architecture the microstructure can be calculated. First it is decided whether Frank-van-der-Merwe (continuous layer) or Volmer-Weber growth (island layer) occurs. The distribution of islands follows a thermodynamic equilibrium approach, which considers the process of island formation while minimizing the free energy of the island surface. The crystallite structure of the matrix material surrounding the islands is calculated by a spatially scaled Potts Modell. The Monte Carlo simulator is initialized with a crystallite structure generated using the Voronoi construction of the crystallite density determined from empirical data using rate equations.

Since volume diffusion is not yet considered, only immiscible multilayer systems can be investigated at present. On the basis of examples, the above-mentioned comparisons are presented.

Author Index

Bold page numbers indicate presenter