Industrielle Gemeinschaftsforschung

Schlussbericht

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Virtuelle Beschichtungsanlage für industrielle Anwendungen (VICIA)

Virtual Coater for Industrial Applications (VICIA)

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Abschlussbericht und Gesamtabschlussbericht

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1. Summary

Due to further optimization and functional integration in coating technology there are continuously increasing demands on deposition processes with regard to complexity, precision, reproducibility on the one hand as well as throughput and cost-efficiency on the other hand. Simulation methods improve the general understanding of such processes and help to minimize the amount of experimental trials for process optimization.

Thin film deposition involves the interaction of manifold mechanisms acting on different size and length scales. A comprehensive multi-physics simulation scheme includes both, the reactor scale process dynamics and the film growth, and has been established in a first version in a previous Cornet funded project »CAPRICe« (Computer Aided process refinement for intelligent coatings). In CAPRICe, a multi-scale simulation chain, namely virtual coater is setup for describing the deposition of TiO_2 layers by reactive sputtering and ion beam sputtering. Four research groups are involved, namely

- Fraunhofer IST, Braunschweig, Germany (IST)
- Laser Zentrum Hannover e.V., Hannover, Germany (LZH)
- University of Namur, Namur, Belgium (UNAMUR)
- CRM group, Liège, Belgium (CRM)

The simulation framework in the former project allowed to model the reactive deposition of TiO_2 layers with the restrictions that the process dynamics model only considers the movement of neutral species and the film growth models only include the growth dynamics for pure metals. Nevertheless, experimental validations shown in [1] were already promising.

In VICIA, the same research consortium extended the virtual coater simulation framework towards more industrial-relevant coating systems, namely multilayered transparent coatings for optical systems and mechanically protective SiO_x coatings for metal working industries; there are the following main advancements:

- The simulation codes for atomistic film growth are improved to handle multiple species and explicitly allow to model the growth dynamics of metal-oxides and interfaces between different coating materials.
- In the process simulation, we developed an additional simulation code for modeling the deposition profile on moving 3D substrates such as optical components. After initial calibration via detailed modeling procedures, this code is real-time capable and can be used for process optimization.
- The atomistic growth simulation now takes into account both, the arrival of neutral species as well as impact of energetic ions from the plasma.
- Besides PVD processes such as magnetron sputtering or ion beam sputtering, a first attempt was made to apply and validate the simulation tools on a PECVD process for SiO_x with a more complex plasma chemical reaction chemistry.

For transfer of the project outcome to the industry, the consortium arranged two hands-on software training workshops together with the user committee. Various successful validation stories prove the general validity and feasibility of the multi physics simulation tool. First subsequent activities aiming to tackle specific coating setups at SME are ongoing.