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Practice-oriented optical thin film growth simulation via multiple scale approach

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ABSTRACT

Simulation of the coating process is a very promising approach for the understanding of thin film formation. Nevertheless, this complex matter cannot be covered by a single simulation technique. To consider all mechanisms and processes influencing the optical properties of the growing thin films, various common theoretical methods have been combined to a multi-scale model approach. The simulation techniques have been selected in order to describe all processes in the coating chamber, especially the various mechanisms of thin film growth, and to enable the analysis of the resulting structural as well as optical and electronic layer properties. All methods are merged with adapted communication interfaces to achieve optimum compatibility of the different approaches and to generate physically meaningful results. The present contribution offers an approach for the full simulation of an Ion Beam Sputtering (IBS) coating process combining direct simulation Monte Carlo, classical molecular dynamics, kinetic Monte Carlo, and density functional theory. The simulation is performed exemplary for an existing IBS-coating plant to achieve a validation of the developed multi-scale approach. Finally, the modeled results are compared to experimental data.

1. Introduction

Modern manufacturing of laser optics is driven by economical and qualitative aspects. This fact led to the development of various coating technologies since the early 1960th. The diverse techniques cover the mentioned requirements to a varying extent, whereat highly economic processes and high end quality procedures are facing each other. Though the production method and the resulting thin film properties are strongly different, their optimization is based mainly on empirical experience. Investigating the growth from a fundamental basis, the development of theoretical models to describe the formation of thin films has moved into the focus.

In order to establish a fundamental understanding of layer growth and to realize a basis for a further optimization of optical thin films, it is intended to develop a theoretical simulation model, which is able to comprise all important processes being responsible for the formation of optical layer properties. The different sequences in the coating plant and the specific growth mechanisms take place on different length scales. Each available atomistic simulation technique is addressed to a selective physical problem and is able to cover only a small range. Therefore, several techniques have to be combined to a multi-scale simulation approach. In order to model thin film formation in a specified coating process, different theoretical methods for the simulation of material generation, the present transport mechanisms in the vacuum chamber, the thin film growth as well as the analysis of the mechanical, optical, and electronic properties have to be merged in a suitable manner. Large-scale simulations, e.g., particle-in-cell Monte Carlo, cover dimensions of several centimeters and are used to model the generation and the transport mechanisms of the coating material inside the process chamber. In contrast, atomistic classical approaches, e.g., kinetic Monte Carlo (kMC) or molecular dynamics (MD), are able to model structures of nanometer size and are applied to simulate the thin film growth in dependence on characteristic coating conditions. It is necessary to note that these approaches have their own advantages and disadvantages. While MD provides a more detailed description of the system, kMC is applicable for longer time ranges and may deal with larger numbers of particles. For this reason, MD and kMC complement each other well. Furthermore, the structural layer properties like film density and surface roughness can be extracted from the modeled layer structures. Finally,

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quantum mechanical techniques, e.g., density functional theory (DFT), are limited to few hundreds of atoms but are well suited to calculate the optical and electronic layer properties of the modeled thin films.

The different simulation techniques were already used isolated from each other to model fundamental topics in modern plasma and thin film technology [1–6]. Consequently, the fundamental experience for the applied simulation techniques is available. The most important issue is the interface between the different simulation techniques. Hence, a main task of the presented study is addressed to the development of the interfaces for the combination of the simulation techniques to a multi-scale model approach.

In the present publication, the discussed model approach is applied to simulate thin film growth in a modern ion beam sputtering, IBS, coating plant. The IBS process is used for the calculations due to several advantages and outstanding characteristics. On the one hand, the IBS technique is known to produce thin films with unrivaled layer quality. This is particularly evident in the dense layers producing a small surface roughness. On the other hand, the IBS process provides a clear separation between plasma interaction zones at the target and at the substrate. This spatial separation simplifies the simulation of material generation and layer deposition. Additionally, the pressure in the IBS chamber is low compared to other common techniques during the coating process, which reduces the computational effort of the transport simulations.

The presented investigations are performed on titanium dioxide, which is a common coating material in many optical multilayer systems. Furthermore, TiO_2 has proven to be an expressive model in classical and quantum mechanical simulations in order to investigate in structural and optical layer properties [7].

The publication is organized as follows. In Section 2, the IBS-coating plant is shortly described. A detailed presentation of the multi-scale approach is given in Section 3, including the different simulation techniques, the developed interfaces, and the IBS simulation results. In Section 4, a comparison is made between modeled data and experimentally achieved results.

2. IBS-coating plant

The subsequently presented multi-scale model is applied to an existing and fully equipped IBS-coating plant located at the Laser Zentrum Hannover e. V. (LZH). By implementing the chamber geometry and the characteristic process conditions into the simulation approach, the evaluated data can be linked to the experimental results of sputtered TiO_2 single layers. The IBS-coating chamber of the LZH is displayed in Fig. 1. The coating plant is equipped with an RIM10 ion source from the University of Gießen and an assistance source from Cutting Edge Coating GmbH. The sputter source is an inductive coupled RF-source with a three-grating extraction system. The source emits an ion current of up to 200 mA, and the acceleration voltage can be varied between 200 and 2000 V. Additionally, the coater is equipped with a load-lock system. The assist source as well as the load-lock chamber are not considered in the performed calculations and are ignored in the direct simulation Monte Carlo (DSMC) approach.

The vacuum system is an oil-free high-vacuum pumping system with a TPH 2301 turbo molecular pump (250 mm flange, 1900 l/s pumping speed). The coating process is operated in a reactive sputtering mode by supply of oxygen through a gas inlet located close to the sputter target. Consequently, metallic and oxide sputter targets can be used for the production of stoichiometric metal-oxide thin films. The coating plant operates with two separate zone targets, which allow manufacturing ternary oxides layers.

3. Multi-scale model approach

In order to combine the large-scale Monte Carlo, the classical atomistic, and the quantum mechanical simulation techniques to a multi-scale model approach, two interfaces are developed. Both secure the data exchange between the different simulation techniques. The task of each interface is to enable the transition between the techniques working on particular length and time scales. Furthermore, they are able to overcome the different limitations of the underlying methods related to the needed computational effort and to realize input data and structures, which can be handled by the subsequent simulation approach. The first interface combines the DSMC and the classical atomistic techniques (kMC, MD), and the second interface enables the calculation of optical properties (DFT) from the classically grown thin film structures by kinetic Monte Carlo and molecular dynamics approaches. In the following sections, the applied simulation techniques as well as the developed interfaces are described in detail in the order of application in the multi-scale approach. Additionally, the simulation results for the example of the IBS-coating plant are given.

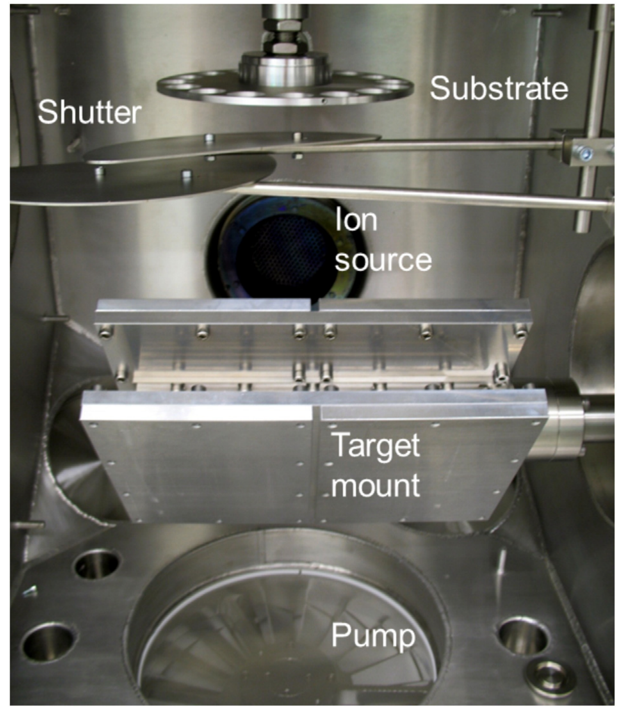

Fig. 1. Investigated IBS-coating plant.

3.1. Direct simulation Monte Carlo

The direct simulation Monte Carlo method is a particle-based simulation technique for the transport of neutral species [8]. It utilizes a statistical approach for solving the Boltzmann equation. The software package developed at the Fraunhofer IST uses massive parallelization to reach feasible computation times for setups like the IBS coater.

The geometry of the chamber is assembled with GMSH, an open-source, three-dimensional finite element mesh generator with built-in pre- and post-processing facilities [9]. The surface mesh of the whole coater is superimposed with a rectangular simulation grid. Each grid cell can contain multiple particles of different species with their positions and velocities. By averaging the properties of several particles, the noise is reduced and general trends of the particle movements become visible. Further parameters like particle density or surface absorption can also be extracted.

For the aim of the combined simulation described in this paper, additional sampling routines are added to the simulation framework. They allow for recording the energy and angular distribution of particles hitting selected surfaces, e.g., the substrate. The obtained energy and angular resolved particle histograms are the basis for later film growth simulations by kMC and MD.

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