Advanced control and modeling of deposition processes

Detlev Ristau[1,2*] **and Henrik Ehlers**[2]

[1] *Centre of Quantum Engineering and Space-Time Research, Hannover, Germany*

[2] *Department of Laser Components, Laser Zentrum Hannover e.V., Hannover, Germany*

[*] *Corresponding author: d.ristau@lzh.de*

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During the last decade, striking improvements could be achieved for the precise control of deposition processes in optical coating technology. For example, as a consequence of enormous progresses in measurement and computer technology, direct optical monitoring in a broad spectral range can be considered as a common tool in many production environments nowadays. Besides the development of the corresponding hardware and measurement channels, advanced approaches for the evaluation of the acquired data and new multiple sensor monitoring strategies moved into the focus of modern research on the way towards deterministic deposition techniques. In this context, also innovative concepts for the simulation of deposition processes to forecast the result for a specified coating design and automatic online correction algorithms gained of importance to reduce the risk of failure in coating production. The present contribution will be dedicated to selected aspects in this field, especially addressing broad band optical monitoring systems. A short review on examples for existing hardware configurations and software tools will be presented illustrating the advantages of modern process control techniques. Novel approaches based on the modeling of thin film growth are discussed as an additional strategy to improve the predictability of coating processes.

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1. Introduction

In strategic technology discussions, the 21st century is often anticipated as the century of the photon with enormous perspectives for the development of mankind. An evolution similar to the development of electronics during the last decades is expected for optical technologies including the creation of integrated optical circuits and systems with highest functionality and efficiency. Presently, lasers and sophisticated optical devices for fundamental research, medicine, space born applications, and industrial production are among the major pacemakers on this technology road. Considering especially the role of optical components, which are the fundamental building blocks of Photonics, ever increasing challenges are particularly imposed on the functional coatings deposited on the surfaces. A clear trend towards demanding specifications not only in respect to quality, precision and complex spectral transfer characteristics covering broad spectral ranges can be observed. Even more, success in the market of optical coatings will progressively depend on the flexibility of the production processes allowing a company to deliver also special coatings in small quantities within short times.

This development calls for a new class of coating processes that enable a deterministic production without time consuming and expensive iteration steps. As a consequence, intensive research on the stability, advanced control, and modeling of deposition processes for optical coatings was performed by numerous groups during the last decade. In the following, a brief review will be given on selected aspects of these extended research activities. After a description of the major ingredients of a deterministic coating strategy, optical monitoring devices, and their combinations with other sensors will be considered. Also, the concept of virtual deposition processes will be discussed on the basis of an implementation with an optical broad band monitor system as an example. In this context, online error detection and corrections tools will be addressed to illustrate the versatility of advanced process control devices. In the final part of the present contribution, a short introduction will be given into new approaches towards modeling of thin film growth to improve the predictability of modern coating processes.

2. Basic components for deterministic coating processes

In Fig. 1, an example for a deterministic optical coating production chain including a virtual deposition process (VDP) simulation[1] and an optical broad band monitoring (BBM) system[2,3] is illustrated. After definition of the customer requirements, the first step comprises the selection of the adequate process, materials and substrates as well as several alternative solutions for the coating design. In the VDP analysis the different designs are evaluated in respect to their expected production yield and possible process instabilities before deposition. The design with highest

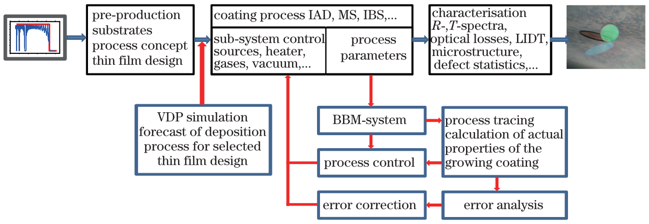

Fig. 1. Production cycle for coated optical components. For the deterministic production of optical coatings, a linear production chain is realised with advanced components for the pre-evaluation of coatings designs (VDP), the control of the deposition process on the basis of optical monitoring (BBM-system) and tracing algorithms as well as error analysis and detection tools.

stability is then deposited under the control of an advanced process tracing tool. In the present example, this online control system is based on an optical monitor directly measuring the transmittance of the growing coating over a broad spectral range. In most cases, the measurement cycles are directly related to the rotation of the substrate holder which defines the time interval between the substrates passing the measurement channel. During each cycle, data are recorded and reduced to calibrated transmission spectra which are transferred to the process tracing algorithm. Within the process tracing algorithm, the momentary thickness of the actually growing layer is determined and compared to the target thickness for layer switching. If the switching point is approached, the algorithm changes to a specially designed time counting mode and generates the switching signal for the deposition plant. In a further expansion stage, the process tracing algorithms is linked to a simultaneously executed program which compares the properties of the produced coating system with the characteristics of the design[4,5]. In case of significant deviations, an error is indicated and a correction tool is initiated which optimizes the subsequent layers to achieve the target transfer characteristics. If no error is detected, the coating process can be completed without operator assistance and results with high probability in a product according to the designed specifications. In this context, the stability of the coating process is of outmost importance for a successful implementation of the deterministic production chain.

2.1 Stable deposition processes

Since most optical monitoring devices directly compare the transfer properties of the calculated design with the layer system growing under typical process environments in vacuum, a variation of the spectral characteristics of the layer system during venting of the process chamber affects the precision of the coating process. Consequently, conventional thermal processes, which often exhibit a vacuum to air shift related to water adsorption, are not well suited for deterministic production processes. However, in the short wavelength range below 240 nm, where fluoride coating materials are predominantly used, the application of broad band monitoring offers advantages in the precision and the quality management of the coating process[6]. For most of the applications in the visible and near infrared spectral range, ion processes in conjunction with oxide materials are preferred due to the achievable dense microstructures with high stability against environmental influences. Ion or plasma assisted deposition processes controlled by optical monitoring have been demonstrated as versatile techniques for a broad variety of products and are available in commercial deposition plants[7]. Similarly, magnetron sputter (MS) concepts in conjunction with optical monitoring have reached a high level of reproducibility and are reported to achieve the deposition of layer systems with several hundred to more than four thousand layers[8,9] covering also complex fluorescence filters[10] or even chirped mirrors for ultra-short pulse laser systems[11]. Ion beam sputtering (IBS) is presently considered as a high quality process with superior stability which is even sufficient for controlling the process in a simple time counting mode for coating systems with modest precision requirements. The small deposition rates of IBS, which are normally rated as the remaining weakness, transform in combination with the low number of pertinent process parameters into an advantage for sophisticated BBM-control techniques. Accordingly, IBS processes gain of increasing importance for the production of high quality optical coatings systems with high precision[12,13] and found also commercialization in adapted deposition systems[14]. New approaches towards flexible IBS-techniques also include the production of coatings from material mixtures with pre-defined contents[15] as well as the accurate realization of rugate filters[14,15].

2.2 Optical monitoring

Nowadays, optical monitoring techniques reach superior precision in layer thickness control and are often favored over quartz microbalance systems which still keep their important position in most deposition systems as standard sensors for regulating the evaporation sources. The history of optical monitoring can be traced back to the late 1960's and documents an enormous development in parallel to the extreme progresses of computer systems in addition to measurement hardware during the last two decades. Both, single wavelength monitoring[16] as well as BBM-techniques[17] could be cultivated to a very high accuracy of layer thickness down to a single atomic layer and to outstanding reproducibility. Modern commercial systems and advanced devices in research comprise direct measurement options, which allow for a measurement of the transfer properties exactly at the product in the rotating substrate holder, and feature self-calibration routines. Self-compensation effects are observed for both methods and are often considered as a major reason for the different performance of the two methods applied to an identical design. From the technical point of view, further progresses in these measurement techniques aim at improved measurement accuracy and spectral resolution. Especially for BBM-systems, the extension of the spectral range would increase the number of available data points and hence, the accuracy of the control system. Other aspects presently investigated concentrate on the simultaneous recording of reflectance and transmittance spectra with adapted measurement channels. In this context, a solution with an Ulbricht sphere has to be mentioned as an interesting approach. In this arrangement[18], the detection system is attached to an Ulbricht sphere which is located near to the substrate holder and significantly reduces the effect of the poor pointing stability typical for the beam reflected by the coating in the rotating substrate holder. Not least, also ellipsometry, which is based on the measurement of the polarization state of test radiation reflected by the growing layer, has been studied for deposition control of dielectric materials[19]. As an innovative concept developed by Masetti *et al.*[20], an ellipsometric system without moving parts in the measurement channel offers advantages for applications in deposition control due to its improved stability to mechanical impacts typical for most deposition systems and reduced data acquisition times. Recent work on single wavelength ellipsometry has been published for an advanced magnetron sputter system[21]. The implementation of spectrally resolving ellipsometric concepts is presently still impeded by relatively long data acquisition times which are only suited for static test glass arrangements.

As a further innovation step on the way towards increased precision of deposition control systems, combinations of different monitoring concepts are presently studied in more detail. In this context, the simultaneous operation of an optical monitoring device in conjunction with a quartz microbalance offers advantages, because the specific weaknesses of the respective techniques are compensated by the strengths of the other method, and both measurement devices can be continuously cross-calibrated during the deposition process. In a course approach, the reliability of BBM-algorithms scales with the integral variation of the spectral behavior during growth of the controlled layer. For example in cases, where a thickness increment of the growing layer induces only a small variation in the recorded spectrum near the noise limit of the BBM-system, the employed fit algorithm may not produce a clear indication of the thickness increment and induce an erroneous switching of the actual layer. This problem can be solved with an additional quartz microbalance which delivers the respective thickness data during the critical phase of the BBM-device, until a stable state of the optical monitoring system is reached again. In this configuration, the BBM-system is channeled through the nondeterministic phase by the quartz monitor and can be employed for switching of the layer with optical precision, which is often higher than the thickness accuracy achievable with a single quartz monitor[22]. Other combinations of control sensors considered for improved process reliability include among others plasma spectrometers, adapted plasma monitors or oxygen detectors.

2.3 Virtual deposition processes

Since the beginning of optical coating technology, the prediction of the stability of a certain coating design in respect to errors occurring during the production was always of major concern. Typical approaches for the estimation of aberrations include the analysis of random variations of the thickness values and the dispersion data of the individual layers within a predefined tolerance band. In corresponding evaluation schemes, the spectral deviations of a large number of designs calculated with randomly varied imperfections are evaluated and allow for an identification of critical layers in the design. However, the forecasts produced by this type of evaluation methods are often observed to be of very restricted utility in practice. Therefore, intensive research work has been concentrated on new, more reliable approaches based on a direct simulation of deposition processes. In these so-called VDPs, the layer growth is simulated by an adequate software producing the virtual measurement signal subsequently processed by the employed monitoring device. The evaluation of the computer-generated measurement data is performed by the software algorithms identical to the program used in the deposition system for the respective monitoring device. Presently available software packages[23] include practical solutions for BBM-systems[22], for single wavelength monitors[24], and also for quartz crystal microbalances.

For illustration of the underlying principles, the scheme of a VDP-algorithm with BBM-control[1] is depicted in Fig. 2. As the fundamental parameter for the process state, a typical thickness increment pertaining to the applied measurement cycle is selected. For the case of the BBM, this thickness step is defined by the time between two consecutive measurements in conjunction with the rate representative for the considered deposition material. The deposition process is emulated by a software algorithm based on the matrix formalisms with input data for the coating design, the deposition material and substrate properties as well as for uncertainties in the deposition stability and coating dispersion. The simulation is started with the calculation of the spectrum for the first thickness increment which is transformed into a set of spectral measurement data. For the derivation of the spectral data a program is used which imitates the measurement channel and takes into account the related measurement uncertainties in respect to transmission, wavelength, and spectral resolution. Then this spectral data set is delivered to the BBM-switching algorithm, which is completely identical to the unit installed at the real deposition and contains a least square fit program for evaluation of the actual layer thickness as well as a routine for comparison of the actual state of the growing layer to the switching point according to the intended coating design. In case the thickness of the actual layer is still far from the projected switching point, the VDP-algorithm continues with processing the next thickness increment. This sequence is repeated until the comparing routine indicates an actual thickness near to the switching point of the first layer. In the following step, the BBM-routine is changed to the time counting mode until the layer termination point is reached. The thickness of the simulated single layer is then calculated as the sum of the last value before detection of the switching point and the additional thickness deposited during the time elapse mode of the

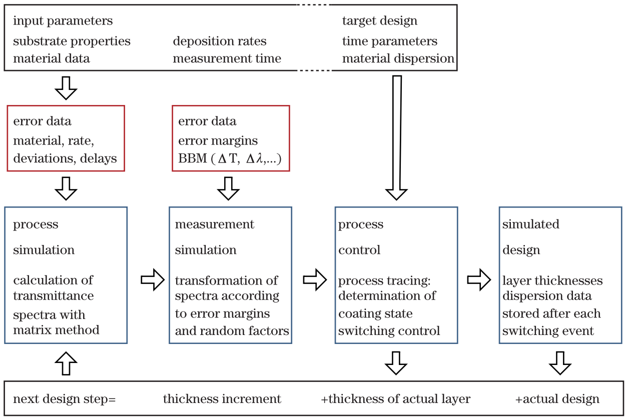

Fig. 2. Diagram for a VDP with a BBM-system for deposition control. The fundamental structure consists of three units simulating the deposition process and the measurement channel of the on-line monitoring device. The process control algorithm is identical to the programme installed in the deposition plant and is also linked to the other program units by the interfaces also employed in the deposition system. The final result of a simulation run is given by the simulated design which is stored layer by layer after each switching event detected by the process control unit.

BBM-routine. This thickness value is stored and the next layer is processed in same way until termination. After treatment of the last layer, the consecutively stored thickness values are considered as the result of the simulation which will vary as a function the parameters and error margins provided to the VDP-software at the beginning of the simulation.

Several studies dedicated to a comparison between the outcome of the VDP-program and the corresponding real deposition runs indicate a very good agreement with the predicted results[1,17]. Hence, VDP-analyses can be considered as a versatile tool to identify problematic designs before the coating process is started and to increase the production yield. As a consequence, VDP-programs gained substantially of importance for industrial production and significantly contributed to an improvement in cost efficiency during the last years.

2.4 Online error detection and correction

Nowadays computing capacities of even standard personal computers reached a level which allows for an analysis of the growing coating system in respect to the target performance during the running deposition process. Consequently, approaches to detect and correct errors during the deposition process, which can be tracked back to 1970's[4], are presently under intensive investigation. Considering a process control system operated with a BBM-device as an example, on-line error detection schemes involve an analysis of the spectra recorded at the termination points of the individual layers and the thickness values of the layers deposited previously. Besides a sequential technique, which calculates thickness deviations only on the basis of the respective spectra at the termination point[5], more sophisticated methods are also examined, which perform an error assessment on the basis of all termination point spectra recorded until the actual state of the deposition process. Recently, investigations in a tool relating multiple spectra were reported[25] demonstrating a higher reliability for ion assisted processes. Since thickness variations alone are not sufficient for an assessment of the running process in practice, an additional calculation step is often included which determines the expected optical performance of the design as deposited. If this computation results in deviations exceeding a predefined tolerance level, the process may be halted or an automatic error correction scheme may be activated. Error correction algorithms can be applied to optimize the remaining layers in the coating design after error detection on the basis of the previously calculated thickness values in respect to the target performance. Advanced algorithms also include a variation of the number of remaining layers to improve the outcome of the deposition process. In the automatic correction mode, the original design provided to the BBM-control system at the beginning of the process will be replaced by the optimized design generated by the correction algorithm, and the process will be continued. In this context, predefined optical performance may not only cover the spectral transmission but also absorption, the phase, group delay, or even group delay dispersion of the coating system. Furthermore, innovative concepts for error correction under investigation comprise an additional VDP-analysis and a variation of the dispersion parameters of the deposited layers. In conclusion, advanced online error correction and detection schemes have been confirmed to improve the stability of deposition processes[5] and can be considered as one step forward to efficient deterministic process strategies in modern coating production.

3. Modeling of thin film growth

Present approaches for the control of deposition processes involve empiric relations between the deposition parameters and the properties of the produced coatings. On the way towards higher flexibility, precision, and quality of coating processes, more sophisticated models for the growth of thin films may gain a key position in optical coating technology. In a visionary picture, novel thin film growth models may close the gap to a fundamental understanding of deposition processes and allow for a direct prediction of the coating properties for a given set of production parameters. Implemented in the production chain (Fig. 1) at the respective links concerning VDP-concepts, processes layout, and control, a new generation of deterministic coating processes may be created. Of course, the present state of the art in thin film growth modeling is still far away from this conception, even though promising developments are under way. In the following, a few aspects of this topic will be discussed before the background of a recent approach on the basis of Monte Carlo methods and molecular dynamics (MD) for the formation of TiO_2 thin films under realistic IBS coating conditions.

For simulations of the time evolution of a given multi atom ensemble, a multiplicity of methods is presently applied to cover different time and length scales. Typical models use either a quantum mechanical approach, i.e., density functional theory (DFT) or classical MD, and kinetic Monte Carlo (kMC) methods[26]. In most cases, classical techniques are employed to consider all processes taking place in the development of dielectric thin films, i.e., deposition, thermal relaxation, surface diffusion and thermal desorption. Georgieva *et al.*[27] had shown that thermally activated surface diffusion can be neglected for the presence of energetic atoms in a growth process similar to the conditions of the magnetron-sputter deposition process. Since the IBS process can be interpreted as a class of sputter techniques and additionally, the classical MD method is best suited to model this energetic deposition process.

The most essential input for the classical MD simulations comprise classical potentials describing all interatomic interactions of the involved species. For this reason, the choice of the appropriate potential is of paramount importance and decides on the quality and validity of simulations. Suitable potentials for a desired combination of materials are derived from adapting a classical potential to the results of ab-initio-simulations[28,29], by fitting to experimental data or by semi-empirical procedures[30]. In the case of amorphous TiO_2[30], an interatomic potential could be adapted to the simple and transferable potential predicted by Matsui and Akaogi[31]. The developed algorithm has been adjusted in a way that the simulated deposition of sputtered target atoms on a substrate is adapted to the real IBS-coating process (Fig. 3(a)). In this approach, the

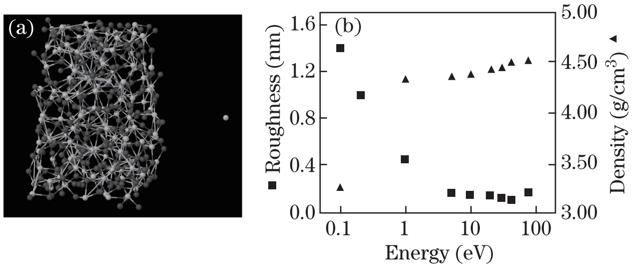

Fig. 3. (a) Simulated deposition of one Ti-atom on an amorphous TiO_2-ensemble; (b) density and roughness as a function of kinetic energy of the impinging atoms.

simulation of each deposition event is subdivided into two different sections. In the first section, the integration of the Newton's equations of motion is done under NVE conditions (i.e., constant number N of particles, volume V, and energy E) to model the energy input in the already existing film. In the second section, the atoms relax under NVT conditions (i.e., constant number of particles N, volume V, and temperature T) in order to cool the thin film down to a given substrate temperature[32]. To investigate in the influence of the specific coating process parameters on the layer formation and structural properties, several simulations were performed using different input values for the kinetic energy, angle of incidence, and deposition ratio. A significant dependence of the achieved film density and surface roughness as a function of deposition energy could be observed (Fig. 3(b)). With appropriate measures for saving computation time, systems up to 4×10^5 atoms could be deposited on a substrate with an area of 14×18 (nm), which in turn corresponds to a film thickness of approximately 18 nm. In addition, to the analysis of structure formation in amorphous TiO_2 thin films, first investigations on alumina using the classical potential predicted by Gutiérrez *et al.*[33] were performed. The realized simulations are in good agreement with the results for titania and show similar dependencies of the structural properties as a function of kinetic energy of the sputtered target atoms. In the next step, the presented model will be extended to the determination of the dispersion behaviour of the materials and will allow for a first forecast of the optical properties of the coatings for selected deposition parameters.

4. Conclusion

During the last two decades, tremendous progresses could be achieved in the evolution of optical coating production. Besides the development of stable ion processes including plasma and ion-assisted deposition as well as concepts of magnetron and ion beam sputtering, enormous impact could be gained from advanced deposition control techniques, effective online correction tools, and novel simulation tools. Nowadays, optical monitoring systems in conjunction with advanced process tracing algorithms have found their way into coating production and are more and more complemented by additional software environments transferred from research to industry. Innovative examples include VDP concepts and automatic error correction schemes, which significantly contributed to an enormous increase in efficiency and production yield during the last years. Research on future innovations in the field addresses combinations of monitoring systems and more sophisticated online correction algorithms. Also adapted models for thin film growth may play a major role in the fundamental understanding of optical coating techniques and the related improvement in coating quality as well as process stability.

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