Using Different Thin-Film Design Software for Different Requirements

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ABSTRACT

The presentation gives a brief overview of the use of thin-film software for the design and assistance in manufacture of thin-film optical coatings, particularly with regard to practical questions and special problems. A shell model will be used to describe which software can be applied for different aspects of design, manufacturing and characterization of optical coatings.

INTRODUCTION

Optical coatings are part of nearly any optics, and their applications range from mirrors for X-rays over dicroic beamsplitters for the VIS up to anti-reflection coatings at terahertz frequencies. Regardless of this very broad spectral range of applications, the mode of operation of all coatings is based on the same straightforward theoretical description. The propagation of light as an electromagnetic wave is described by Maxwell's equations and there are suitable solutions describing the effect of optical coatings, for example based on the so-called matrix formalism [1]. But this formalism provides only the description of the spectral performance of an optical coating and questions remain as to how to get the corresponding design for a desired application and how to manufacture such an optical coating. Answering these questions is strongly connected to suitable technologies for the deposition of thin films and a number of measurement devices and methods. But there is also great demand for suitable software to simulate all the effects and to solve all the problems connected with the design, the manufacture and the application of optical coatings. In this sense, progress in thin-film optics is strongly connected not only to deposition technologies but also to progress in computer hardware and software.

The next section reviews known thin-film software tools by means of a straightforward shell model of the required thin-film software (Figure 1). Different shells for analysis, analysis expansion, design assistance, design transformation, synthesis, system integration, manufacturing assistance, and monitoring simulation are listed and briefly described. Some of the examples presented are taken from topical applications of optical coatings. In conclusion, the shell model is used to review the progress in thin-film optics over time, characterizing the state of the art in thin-film optics and referring to some future developments.

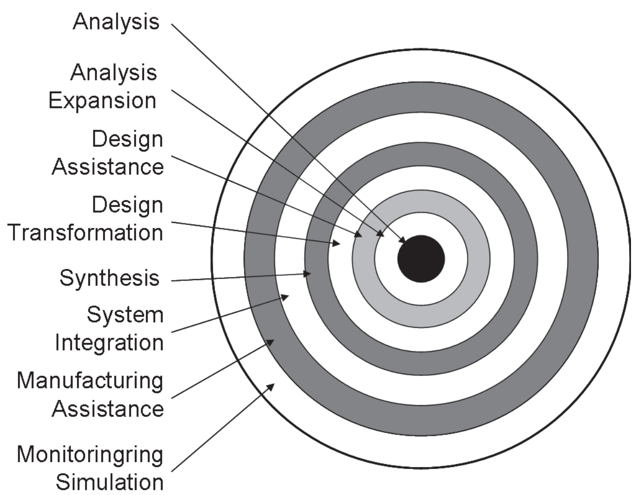

Figure 1: Shell model of thin-film software components.

SHELL MODEL OF THIN-FILM SOFTWARE

Analysis

The theory of optical coatings is a well-defined and self-contained theory, and everything about it has been experimentally proven. Assuming a given coating design as a solution for a desired optical performance, the spectral and angle-of-incidence-dependent performances can be easily analyzed using matrix formalism or a similar procedure [2]. Anyone can apply this formalism using the simplest model of a programmable computer and any commercial thin-film design software contains this procedure as a core tool. In this sense, analysis can be understood as the core of a shell model of thin-film software.

The input for the design analysis is given by a so-called environment that refers to the refractive indices of incident medium and substrate and the angle of incidence of the incoming beam, the design itself and the data of the materials used. In the sense of a core tool, the output analysis is any type of spectral performance, and these performances can be checked under different parameter values or different environments, and between different database designs. One commercial thin-film design software provides a special 'interactor' tool which helps to visualize the principal performance of an optical coating [3].

 505/856-7188
52nd Annual Technical Conference Proceedings, Santa Clara, CA, May 9–14, 2009 ISSN 0737-5921

Analysis Expansion

Optical coatings affect the propagation of a light wave also in dependence on the physical thickness of the coating itself. The thickness defines a time duration of the light wave within the coating which becomes important in modern optical applications including ultrafast lasers. In general, lasers as light source require the consideration of special effects within the coatings and this provides the justification for an 'analysis expansion' shell. Expansion means that there are additional sets of formulas to calculate special parameters as in the field of laser applications, such as the Group Delay, Group Delay Dispersion, and Third Order Dispersion. Meanwhile, such special software tools are included in commercially available design software.

Analysis expansion can also be understood as a requirement for a formalism to consider the diffraction of light within a laterally modified optical coating. Such an expansion is required in the description of equivalent refractive indices given by a relief-structured surface for the application of anti-reflective coatings similar to the moth-eye structure. In such a case, the analysis has to be expanded using the Rigorous Coupled Wave Theory to extract solutions that additionally involve a change in refractive index in a direction that is vertical to the propagation of the light wave [4].

Simulating the color of an object whose surface is modified by an optical coating can be seen as a well-known example of the expansion of design analysis. Any thin-film software provides a tool for coating color calculations with the aim of numerous special definitions around the color, such as different color coordinate systems, different observers, color matching functions, and standard light sources. A typical example for the application of analysis expansion by the color tool is the application of notch filters in ophthalmologic surgery systems (Figure 2).

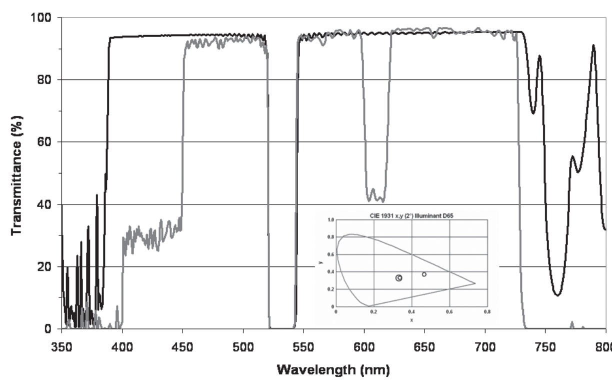

Figure 2: Transmittance of a color-corrected 532nm Notch-filter (grey) with x,y-color-coordinates x = 0.33 and y = 0.33 (dobble-circle within the embedded diagram), and an uncorrected 532 nm Notch filter (black) with x,y-color coordinates x = 0.46 and y = 0.36 (single circle within the embedded diagram).

Another aspect of analysis expansion considers possible non-optical properties and some problems for later spectral measurements. For example, the cone of light incident on a sample in a spectrophotometer gives a range of angles of incidence on the sample surface and the spectral performance of the coating is averaged over the cone angle. In the case of very narrow band-pass filters or of very steep edges of longwave-pass or shortwave-pass filters, this effect directly influences the spectral performances. The bandwidth of the slit through which the radiation enters and leaves the monochromator of the spectrophotometer has similar influence, because the width of the slit smoothes the spectral characteristic. Both effects can be the source of some differences between the theoretically evaluated and the measured spectra and both effects can be simulated by special software tools.

Design Assistance

The theory of thin-film optics provides the designer with formulas and formalisms that are tailored to functionally determined problems or special design types, respectively. Assistance is required in creating such special design types, which leads to the name 'design assistance' for this model's shell. Typical examples of such design assistance are the submenus for creating thin-film optical filters such as band-pass filters and induced transmission filters.

Another example of design assistance close to modern applications is the design of a rugate filter. This type of thin-film optical filter is characterized by a sinusoidal profile of its refractive index versus physical thickness, and its spectral characteristic can be derived using an explicit formula. Such a profile allows the realization of a spectral characteristic including very broad bands of high transmission but very small bands of high reflection. At present, the progress in thin-film technologies allows the realization of special rugate filters that create the possibility of increasing the known laser damage thresholds to unexpected values [5].

Design Transformation

Beyond design analysis and design assistance, there is an application of the Fourier Transform method for the design of optical coatings. This is an obvious approach because both wave number and optical thickness are variables of the phase thickness of any thin-film arrangement [6]. Because the application of the Fourier Transform method is not restricted to the creation of special design types, this design transformation is more than design assistance but it is not yet the known design synthesis. In this sense, it represents its own 'design transformation' shell in the used model. However, there is no commercially available thin-film design program which includes the Fourier Transform method, so one has to use suitable scientific programs [7].

Synthesis

If analysis, design assistance and transformation are not sufficient to create the required design for a given application, other formalisms are required, in principle. The next shell of the model includes synthesis as a general requirement to develop a coating design that fulfils any spectral characteristic or any specially defined optical performance without the need for deeper knowledge in thin-film optics on the designer's part. Design synthesis uses known optimization procedures similar to those that have been developed for the solution of general engineering problems such as Nonlinear Simplex, Newton, Simulated Annealing, or Damped Least Squares, as examples [8].

As input for design synthesis, a target has to be defined based on the required optical performance. Furthermore, constraints have to be considered concerning the minimum layer thicknesses or available refractive indices, for example. And finally, a suitable figure of merit is used to drive the changes in the optimization parameters and to indicate when a satisfactory solution has been reached. In an initial approach, a refinement procedure is used for the improvement of the performance of an already existing design. In any case, after refinement there is a remarkable performance improvement with respect to the defined target, but the given design restricts possible better solutions by its layer number and overall thickness.

Applying an evolution of the design in its layer number and overall thickness seems to be a better approach to synthesis. There is a simple model of a synthetical approach concerning the optical thin-film specificity: The spectral characteristic of any optical thin-film design is based on the interference effect and this effect itself is based on the phase difference of at least two different beams within the coating and with respect to its environment. Adding layer onto layer into a design enlarges the number of possible phase differences. The more phase differences are available, the more interference takes place and the more details within the spectral characteristic of the coating can be realized. If adding a layer is performed using a very thin layer, this method is called the Needle method and the corresponding software is one of the most powerful thin-film synthesis software options [9].

System Integration

In the end, any optical coating is part of an optical system that defines a number of requirements on the coatings, and these requirements call for special software tools that result in a 'system integration' shell. Usually, the optical system contains a series of coated surfaces, and some software allows the calculation of the spectral performance of an assembly of coatings and substrates, called, for example, vSTACK [10]. The optical system design also involves a number of other aspects that influence the spectral performance of the coating. The light source provides a wavelength-dependent illumination or the detector provides a wavelength-dependent sensitivity, and both effects can be considered in the coating's design. And finally, a complete optical system is analyzed by typical system design software as ZEMAX or OSLO, which requires corresponding considerations for exporting the coating designs.

Manufacturing Assistance

The more challenging the optical performance of an optical coating, the more assistance the deposition process requires using suitable software, hence the name 'Manufacturing Assistance' for the shell in the model used. Two types of assistance can be distinguished: Tools that are still part of the design program after a design has been completely optimized, such as Tolerancing, Layer Sensitivity, and Monitoring Curve; and tools that can be seen as part of the plant control software because they consider some of the deposition and measurement parameters and their errors.

The simulation of layer sensitivity lets the designer determine which layers are most sensitive to thickness errors. The so-called tolerancing varies the thicknesses of layers randomly or systematically, and analyzes the design performance based upon these errors. Small changes in a layer's thickness can lead to a large increase in the value of the figure of merit or to a modification of the spectral performance, which in both cases eventually puts the coating run at risk. The monitoring curve program calculates the transmittance or reflectance at a single wavelength and simulates an optical monitoring in principle [11].

Except for some simple coatings made by sputtering or spin-coating technologies which are controlled merely by time, most deposition technologies of optical coatings are controlled by the aim of a quartz crystal, an optical monitoring system, or sometimes both. For these monitoring systems, a so-called runsheet is provided which contains all the information needed to control the deposition process with respect to the coating design. If the deposition process runs normally, the simulated errors do not all appear obviously. But there are design types that make it possible to realize the required performance of the coatings in spite of typical process errors in a layer's thickness. For designs consisting of layers of equal optical thicknesses and even multiples of this thickness, there is an error compensation effect which suppresses the accumulation of thickness errors and leads to surprising precision in manufacturing [12].

But there are also critical designs generating on-line spectral monitoring data, which can be misinterpreted during the deposition process. As a consequence, large deviations in the layer thickness occur, or, in the worst case, a failure to identify the layer termination point may occur and the deposition process ends in a condition that cannot be corrected. To overcome these problems, broadband monitoring systems (BBM) have been developed and introduced in the daily manufacturing process assisting the deposition process in a novel matter [13]. One of the monitoring concepts is based on the determination of the actual thickness of the growing layer on the basis of the transmittance spectrum measured at tact during the deposition. The actual thickness of the growing layer is updated after each revolution of the calotte, allowing for precise control of the deposition process in the dimensions of half a nanometer [14].

If the coating is eventually manufactured, a re-engineering program based on the refinement program can be used to identify real errors in thickness and refractive index made during the manufacturing process. This gives feedback for the evaluation both of the chosen design and the quality of the manufacturing process used.

Independent of the latest measurement tool for the on-line control of layer thickness, an essential part of any manufacturing assistance is the database of the materials used. This database is defined by the refractive index and the extension coefficient in dependence of the wavelength of all the materials that can be used for the coating designs with regard to their spectral range of application. Because the optical parameters of the material depend directly on the deposition technology used, the parameters must be determined from time to time or after changing essential deposition parameters. Most thin-film design programs also provide the designer with some tools to extract these parameters using experimental results of single thin films, but there is also a program that combines optimization and synthesis design capabilities with powerful tools for analyzing spectroscopic and ellipsometric data of single thin films [15].

Monitoring Simulation

Meanwhile, most thin-film design software provides special simulators which have the capability of modelling the behaviour of the monitoring system used. At first glance, such a monitoring simulator seems to be more a computer game than a helpful device for controlling the deposition process. However, the simulators allow for the consideration of nearly any possible error of each of the used parameters, as for example, the light source noise level, temperature effects, signal, and wavelength errors. For each of the errors, the mean value and the standard deviation can be considered.

The connection of simulating errors of individual layers of the design used as well as errors of the monitoring systems allow the designer and the process operator to check the deposition process preparation and to minimize the impact of possible errors. For example, in some cases the optical monitoring strategy includes changing the monitoring chip and the simulator helps to accomplish this before the deposition process is out of the target (Figure 3).

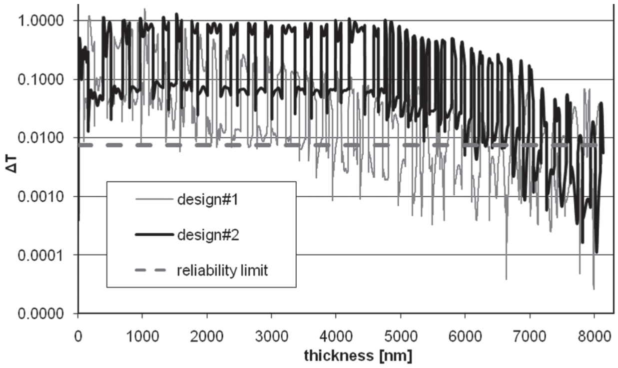

Figure 3: Monitoring ΔT-function of two different TiO_2/SiO_2 non-quarterwave designs, each with a total thickness of 8.5 μm, in comparison with the reliability limit of the ΔT-function, which indicates a necessary change of the monitoring chip [14].

CONCLUSIONS

Reviewing the use of thin-film software and special components of such software shows a number of tasks, problems and effects that occur surrounding the design and manufacture of optical coatings. Under the aspect of requirements that must be fulfilled by the optical coatings and their manufacturing, it is possible to separate these software components into different groups. The arrangement of these components into a shell model renders all core components of the software clearly visible and indicates the progress during the manufacture of optical coatings. The shell model also seems suitable for tracing the development in the field of optical coatings over the time, in this case as driven by the progress in the software used and its hardware. Usually, theory waits for the necessary software, as in the case of the Needle method, which was developed theoretically in the 80s and was only realized as powerful hard- and software at the beginning of the new millennium. But practice was waiting for the necessary software as well, as in the case of rugate filters which can be described very simply theoretically and are now realized practically with unexpected performance, by the means of broadband monitoring and its simulation.

The shell model visualizes the need for considering all the inner shells if, for example, someone works in the field of the monitoring simulation as an outer shell of the model. The shells also visualize the complexity of optical coatings and their manufacture. Considering all the shells, it seems feasible to fulfill all the wishes of an optical system designer for the optical coatings, and, understanding the design analysis as a core requirement, the possibility of using real-time design analysis seems feasible in the future. If the individual layers are measured in thickness and refractive index during the deposition process, it appears possible to adjust the thickness of the remaining layers of the coating if any error at an individual layer is indicated by the monitoring system. Such a type of completely automatic coating process has not yet been implemented in a commercially available coating plant, but it is in development and demonstrates the future in thin-film manufacturing, based not only to the progress made in the deposition technologies but also in thin-film software. However, any type of automatic design and manufacturing does not reduce the need for comprehensive knowledge and skill in thin-film optics, both in theory and in practice.

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