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A hybrid algorithm for reengineering the refractive index profile of inhomogeneous coatings from optical in-situ broadband monitoring data

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Abstract : Reengineering the refractive index profile of inhomogeneous coatings is a troublesome task. Multiplicity of solutions may significantly reduced by providing additional information. For this reason an in-situ broadband monitoring system was developed to measure the transmittance of the growing film directly at the rotating substrate. For characterization of these coatings, a new model was developed, which significantly reduces the number of parameters. The refractive index profile may be described by a proper number of equally spaced volume fraction values using the Bruggeman effective media approach. A good initial approximation of the refractive index profile can be generated based on deposition rates for both materials recorded with quartz crystal monitor during manufacturing. During the optimization process, a second order minimization algorithm was used to vary the refractive index profile of the whole coating and film thickness of the intermediate stages. Finally, a significantly improved accuracy of the modelled transmittance was achieved.

Key words : inhomogenenous coating; refractive index profile; broadband monitoring; hybrid algorithm

1　Introduction

Inhomogeneous coatings with a well-defined continuous refractive index profile along an axis that is perpendicular to the film surface, such as so-called gradient index layers and rugate filters represent new and prospective thin film designs. Particularly, the low optical scatter level and the wide accessible angular range make them superior to traditional stacks with respect to selected applications such as notch filter or omni directional devices[1]. Manufacturing such systems in practice requires new synthesis, adapted deposition processes and improved methods for monitoring and characterization.

The Leybold Syrus Pro 1 100 deposition system can be used to manufacture inhomogeneous coatings by co-evaporation of SiO_2 and Nb_2O_5[2-3] Additional information on the intermediate stages of the not yet completed film is extremely helpful in reverse engineering tasks, and clearly superior to the extent of information that may be drawn from the spectra of the completed film only. That information may be collected by measurements of the transmittance of the growing film directly at the rotating substrate with our in-situ broadband monitoring system (Fig. 1).

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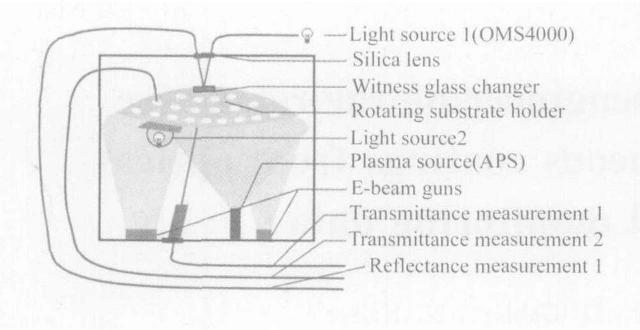

Fig. 1 Experimental setup for in-situ broadband monitoring and deposition of inhomogeneous coatings

2 Algorithm

To achieve a fast convergence of the reengineering algorithm, a good start approximation and proper model are required. In the case of depositing inhomogeneous coatings by co-evaporation, technological problems result in significant discrepancies even between designed and manufactured deposition rate profile (Fig. 2).

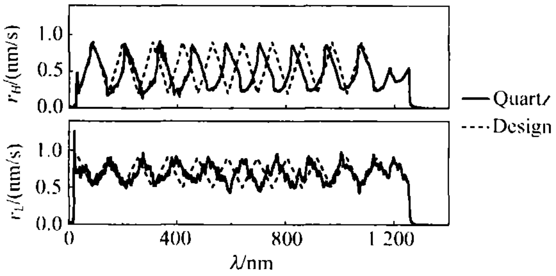

Fig. 2 Recorded with quartz crystal monitor (solid) and designed (dashed) deposition rates of Nb_2O_5 (top) and SiO_2 (bottom)

In particular, these discrepancies may be reduced if time delays during the deposition process are taken into account (Fig. 3). Systematic derivations of the deposition rate profile of Nb_2O_5 are caused by thermal inertia of the crucible. Additional, accumulated time delays results in erroneous control behaviour of the deposition process at the end. For this reason, the recorded deposition rate profile will be better suited to generate a good start approximation of the refractive index profile than the original design.

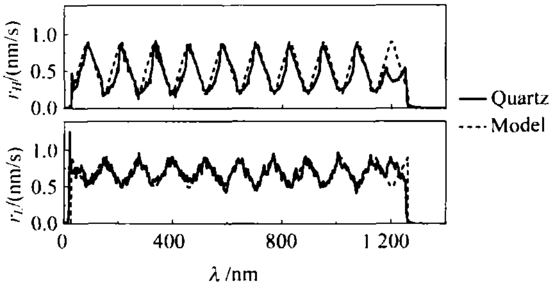

Fig. 3 Recorded with quartz crystal monitor (solid) and modelled (dashed) deposition rates of Nb_2O_5 (top) and SiO_2 (bottom)

The physical thickness z of the coating at any given time t can be estimated by integration the sum of the both deposition rates:

$$z(t) = \int_0^t r_L(\tau) + r_H(\tau)\,\mathrm{d}\tau, \qquad (1)$$

The volume fraction p of Nb_2O_5 at a given time can be also estimated from the deposition rates:

$$p(t) = \frac{r_H(t)}{r_L(t) + r_H(t)}, \qquad (2)$$

Using these two equations, the volume fraction profile $p(z)$ is given in parametric form. The number of points in the resulting volume fraction profile depends on the time resolution of the deposition rate recording. To keep the number of parameters as low as possible, the volume fraction profile can be smoothed to eliminate noise. Small inhomogeneities with thicknesses of only a few nanometres do not affect the transmittance in the visual spectral range and can be neglected. For this reason, the volume fraction profile can be transformed into step function with equal optical thickness (Fig. 4)[4]. Thereby the step length for the inner steps was kept constant and set to twice the value for the first and last step. In this case, the step profile of the volume fraction can be finally transformed into a piecewise linear profile with equally spaced values (Fig. 4). This approach significantly reduces the number of required parameters for the volume fraction profile.

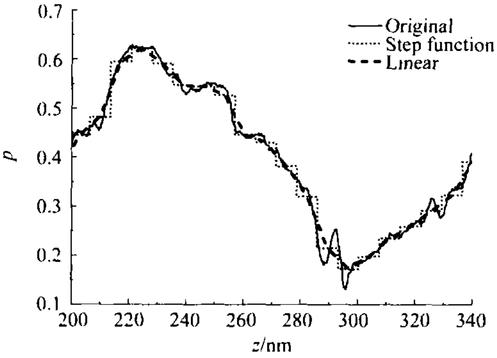

Fig. 4 Smoothing the volume fraction profile (solid) significantly reduces the number of parameters. A step function with equal optical thickness (dotted) can transformed into a piecewise linear function with equal spaced sampling points (dashed).

For modelling the refractive index profile based on the volume fraction profile a mixture model is required. For a homogeneous mixture, where the constituents cannot be classified into inclusion and host, the Bruggeman's mixing formula can be used[5]. For any given wavelength, the complex refractive index profile of the mixture $\hat{n}_{\mathrm{eff}}$ can be calculated from the complex refractive indices of the individual film constituents SiO_2 ($\hat{n}_L$) and Nb_2O_5 ($\hat{n}_H$) and the volume fraction profile p:

$$\hat{n}_{\mathrm{eff}} = \frac{1}{2}\sqrt{(3p-1)\hat{n}_H^2 + (2-3p)\hat{n}_L^2 \pm \sqrt{((3p-1)\hat{n}_H^2 + (2-3p)\hat{n}_L^2)^2 + 8\hat{n}_H^2\hat{n}_L^2}} \tag{3}$$

This refractive index profile can be used to model the transmittance of the coating. For all I in-situ transmittance spectra, each containing J spectral points, the same equidistant volume fraction profile ($p_0 \ldots p_m$) must be valid. Only thickness d of the sub-system may vary. For this reason, the merit function can be defined as:

$$F(p_0 \cdots p_m, d_1 \cdots d_I) = \frac{1}{I}\frac{1}{J}\sum_{i=1}^{I}\left(\sum_{j=1}^{J}\left(T_i(p_0 \cdots p_m, d_1 \cdots d_I, \lambda_j) - T_i^{\mathrm{insitu}}(\lambda_j)\right)^2\right)$$

average of the squared difference between modelled and measured transmittance. Fig. 5 illustrates the good qualitative agreement between in-situ measured transmittance (symbols) and start approximation (solid line). The stop band is shifted approximately 7 % in wavelength, which results from a higher optical thickness of the deposited rugate filter. During the optimization process, the physical thicknesses were first adjusted to reproduce the position of the stop band. This significantly reduces the value of the merit function without changing the refractive index profile and improves stability of the optimization process.

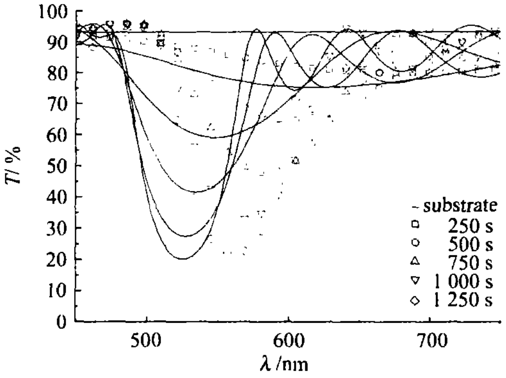

Fig. 5 In-situ measured transmittance (symbols) and start approximation (solid lines)

Finally, a second order optimisation algorithm was used to adjust the volume fraction profile and the thicknesses of the particular coating at the time of the in-situ measurement. In comparison to the number of variables (a few hundred) the required number of optimization cycles to achieve a good agreement between model and measurement was low (approximately 50). The parameters of the model reproduce the position and width of the stop band as well as the optical behaviour of the coating in the side-bands even for intermediate states of the deposition process (Fig. 6). This indicates that the extracted parameters does not only represent a possible mathematical solution of the reengineering task but also contains important physical information.

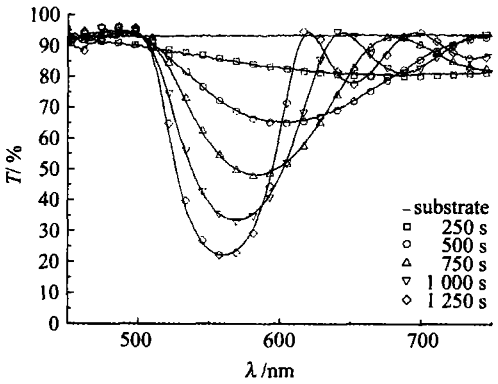

Fig. 6 In-situ measured transmittance (symbols) and final result of the optimisation (solid lines)

In Fig. 7 the calculated refractive index profile at 600 nm is shown (solid line). The physical thickness of the coating is more than 10 percent higher than expected. The shape of the envelope of the final result is similar to the envelope of the start approximation (dotted line). The minimum and maximum refractive index values of the calculated refractive index profile are shifted to lower values and result in a lower average refractive index of the coating.

For this reason, an adjustment of the deposition rate records is required. The simplest approach is given by modified tooling factors. Unfortunately, this doesn't completely explain the calculated refractive index profile. In a more advanced approach, the cross talk between the two quartz crystal monitors must be taken into account. Based on the geometrical conditions in the deposition system, each quartz crystal monitor particularly detects also a fraction of the signal of the other one. This may considered by using a 2 × 2 matrix to modify deposition rates. In this matrix, the diagonal elements are the tooling factors and the non-diagonal elements describe the cross-talk. Applying this model to the start approximation, an improved start approximation can be calculated (Fig. 8, dotted line). There is a good accordance between the reengineered refractive index profile and the improved start approximation. The determined cross-talk of SiO_2 to Nb_2O_5 quartz crystal monitor is approximately 5 %. For the opposite direction, no cross-talk must be taking into account, because a pipe in front of the SiO_2 quartz crystal monitor completely shields this crystal from Nb_2O_5.

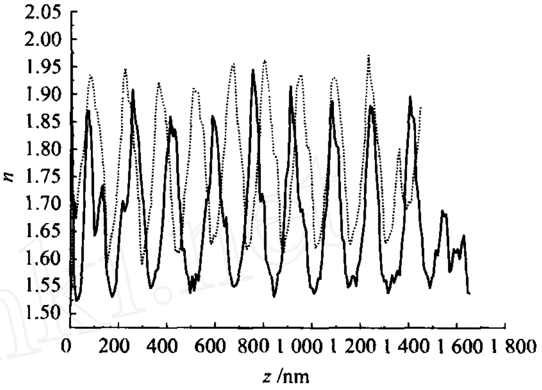

Fig. 7 Reengineered refractive index profile (solid line) and start approximation (dotted line) for a wavelength of 600 nm

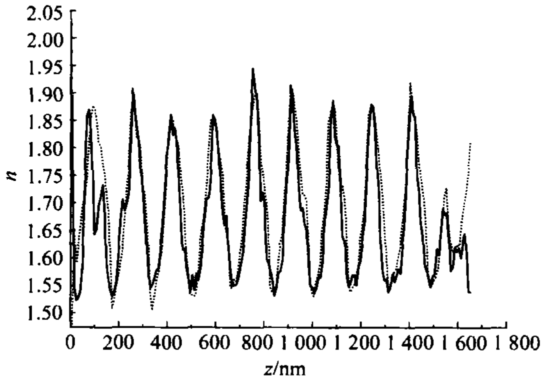

Fig. 8 Reengineered refractive index profile (solid line) and improved start approximation (dotted line) for a wavelength of 600 nm

3 Summary

A new algorithm to reengineer the refractive index profile of inhomogeneous coating from in-situ measured transmittance on the rotating substrate was developed. The refractive index profile may describe by a proper number of equally spaced volume fraction values using the Bruggeman effective media approach. A good start approximation of the refractive index profile can generated based on deposition rates for both materials recorded with quartz crystal monitor during manufacturing. This may further be improved, when cross-talk between the quartz crystal monitors is taken into account.

During the optimization process, only the volume fraction profile of the whole coating and film thickness of the intermediate stages were modified. This restricts the multiplicity of solutions. Finally, a significantly improved accuracy of the modelled transmittance was achieved. The shape of the reengineered refractive index profile is consistent with recorded deposition rates.

4 Acknowledgments

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Brief professional biography of the author:

Stffen Wilbrandt, male, native of Jena in Germany, was born in January 1972. He completed his graduate in physics in 1998 at the Chemnitz University of Technology and is currently a PhD student and scientific co-worker at the Institute of Applied Physics, Friedrich-Schiller-University Jena. He is investigating in the field of design, monitoring and characterization of homogeneous and inhomogeneous optical coatings.