Process Design Issues for Rugate Coating Fabrication

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ABSTRACT

Rugate coatings are optical interference films where the refractive index of the film continuously and periodically grades as a function of the film's optical thickness. The required index variation is typically achieved by co-depositing two materials of different refractive index. Co-deposition complicates process monitoring and control. Bleed gas rates for reactive deposition processes and ion beam parameters for IAD processes must be actively controlled as the constituent material rates are varied to ensure good process quality. Blended material systems are more sensitive to temperature and source plume distributions than are discrete stack filters. Undamped ringing in proportional-integral-derivative (PID) controllers for source rates and temperature can lead to degradation of out of band transmission in the filters. The challenge of fabricating rugate filters is not so much filter design, as it is process design.

In this paper, we discuss issues of concern in designing a rugate process. We present control and monitor methods that have been implemented and suggest areas where improved process capability in commercial controllers would aid development of this emerging technology.

INTRODUCTION

Rugate films offer several distinct performance and manufacturing advantages over current discrete stack film technology and are particularly suited for broadband and multi-band spectral applications. The index profile of a complex, high performance design is quite challenging to fabricate and process monitoring and control are the keys to success. Rugate filters of nearly all spectral types—narrow notch reflectors, bandpass filters, cold shield filters, polarizing and non-polarizing filters have been fabricated using a variety of processes.

Optical interference filters have been traditionally fabricated by depositing successive layers of materials of different refractive index. A simple notch reflector can be fabricated by depositing successive layers of high and low index materials. The bandwidth of the reflection notch is a function of the index contrast or difference between the high and low indices. Discrete filters will typically exhibit multiple reflection bands at harmonic wavelengths of the principle reflection notch. Over the years, numerous design techniques have been developed to suppress specific harmonics, produce limited broadband performance and better optimize discrete designs. However, as optical systems become more complex, the spectral demands on the optical filters in these systems have also increased. The rugate filter was conceived as a means of simplifying the design of complex films by utilizing state of the art manufacturing processes, in-situ monitoring, and process control technologies.

Rugate filters were originally conceived as a means of providing narrow reflection notch filters. It was proposed that by varying the index profile sinusoidally, rather than as a square wave, and by controlling the index excursion, very narrow notch filters could be produced [1]. Further, since the sine wave index profile is free of higher order harmonics, multiple index profiles could be easily superimposed to produce complex spectral performance. Today, a variety of basic waveforms are used to design rugate filters, but the sine wave continues to be the most versatile. The profile follows the form:

$$n=n_a + n_p/2 \sin (4\pi/\lambda \, . \, n_a * z + \phi)$$

where n_a is the average index, n_p is the index excursion, λ is the reflection wavelength, and z is the current thickness [8].

Figure 1 illustrates the key parameters which describe the sinusoidally varying index profile of a single notch reflection filter. The optical thickness period of the sine wave variation determines the location of the reflection notch. The amplitude of the sine wave is determined from the desired bandwidth of the notch and the average index of the film system. The optical density of the notch is a function of the amplitude and the number of rugate cycles.

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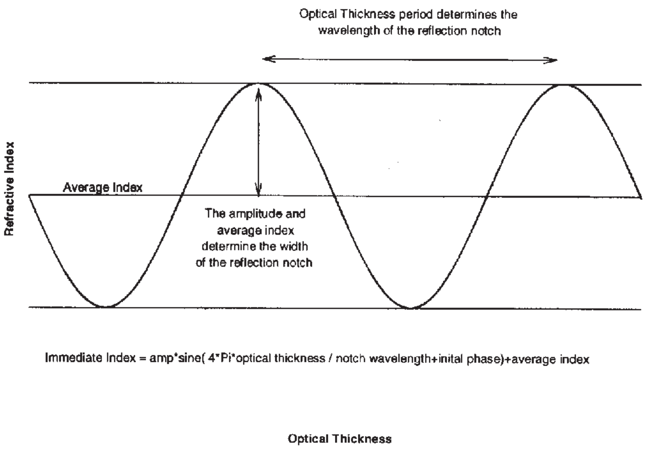

Figure 1. A Rugate interference filter requires precise control of refractive index as a function of optical thickness. In the case of a simple, single spectral notch reflection filter, the index of refraction is varied sinusodually. The width of the notch is a function of the index amplitude and the wavelength of the notch is a function of the optical thickness period. Optical density of the notch is a function of the number of rugate cycles and the amplitude.

PROCESS DESIGN ISSUES

Process design, monitoring, and control are key to the successful fabrication of high performance Rugate and discrete filters. A visible narrow notch filter can be 20 to 30 microns thick and require 6 to 20 hours of deposition time depending upon the design and process. Infra-red filters are typically 3 to 5 times this mechanical thickness. Refractive index profiles range from the fairly simple profiles required for gradient index anti-reflection films to the complex profiles required for multi-band filters. Figure 2 and Figure 3 illustrate this point by showing the index profile required for a four-notch visible filter fabricated by superimposing the profiles for each of the individual lines and the resulting spectral performance.

Even the most stable of processes require monitoring and active correction for parameters such as source depletion, changes in source plume, and degradation in process equipment. Precise and timely control of immediate parameters such as layer thickness, material rates, substrate temperature and backfill gas rates must be consistently monitored throughout the deposition.

Table 1 list a number of parameters which impact the optical performance of the final film. An estimate of the time period over which active control becomes critical is listed under measurement rate. Generally speaking, precise control of the optical thickness of the cycle or group is most critical as it determines the location of a reflection notch or pass-band. For a Rugate filter, the waveform is critical in determining the presence or absence of higher order harmonics, side-lobe structures, notch bandwidth, and out of band transmission. If co-deposition is used to generate the continuously varying index profile, then precise control of both material rates is required. For discrete films, precise control of the optical thickness of each layer is required. Material rates are much less important for discrete films, although excursion in rate will effect film density, and hence the index of the film.

Successful deposition requires the monitoring and correction for long term process variability due to source depletion and equipment degradation as well as control of immediate parameters such as deposition rates and substrate temperature.

Any index within the available contrast range of materials, in any combination, is theoretically possible with co-evaporation. The challenge is how to fabricate these new designs, and the keys to success lie in the selection of materials, depo-

Table 1. Design, Monitor and Control Parameters

Design Parameter	Measurement	Measurement Rate	Performance Impact	Comment
material rates	crystal rate monitor	1/sec	waveform control	controls mixing ratio
Optical Thickness/ cycle (OT)	monitor signal turning point	1 to 5 minutes	reflection notch position	end of cycle/group reset
Amplitude (index contrast)	OD/cycle, OD variation	1 to 5 minutes	notch bandwidth, side lobes	blending ratios and material density
cycle to cycle coherence	cycle to cycle phase	1 per cycle	edge slope, poor OD/cycle	on-band monitor
Optical Density of notches (OD)	number of cycles/ groups	1 to 5 minutes	film thickness	on-band monitor
Average index	bandwidth	1 to 5 minutes	field of view	broadband monitor
periodic errors	RMS PID output	5 sec	unwanted reflection bands	broadband monitor
long term trends	OD growth/cycle	0.5 to 20 hours	poor out of band transmission	off band monitor

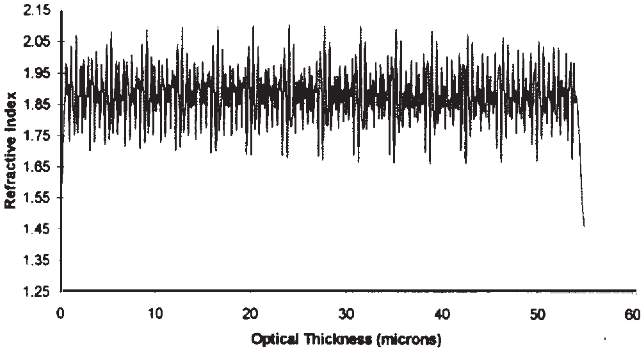

Figure 2. The refractive index profile for the four-line visible notch filter shown below.

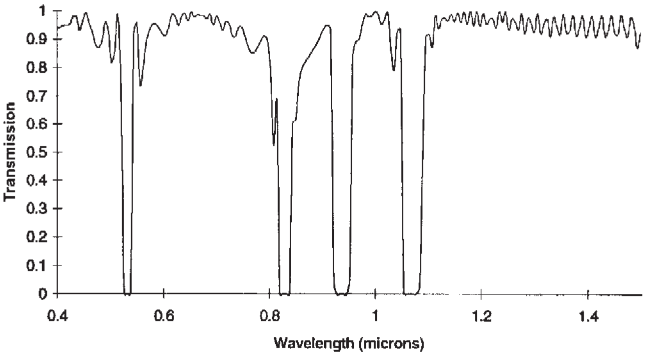

Figure 3. Predicted spectral transmission for the notch filter designed in Figure 2.

sition process, process monitoring, and control techniques. Co-deposition of two materials is the most commonly used method although modulation of gasses in reactive deposition of single materials or mixed solid solutions shows promise [9]. A typical visible application uses TiO_2 and SiO_2 evaporated out of electron guns. An oxygen bleed gas is added to allow for reactive deposition.

PROCESS DESIGN METHODS

Numerous methods have been proposed and implemented for rugate process control [4]. The principal commercial means of controlling deposition processes is the use of quartz crystals to measure deposition rate, and single wavelength, single point optical monitors. Quartz crystal monitors relate the change in oscillation frequency of a thin, water cooled, quartz crystal to the mass of the material being deposited. The crystal measures change in mass on the crystal, and, as such, does not directly yield information of relevant optical properties such as optical thickness, refractive index or film density. Since the crystal must be water cooled, the deposition rate it measures can be very different from the deposition rate on heated substrates of different materials at other locations in the chamber.

Table 2. Estimates of current commercial insitu methods are compared with the required control accuracy, illustrating the need for improved process control sensors.

Physical Property	Typical Range	Current Insitu Capability	Control Accuracy Needed	Comment
Mechanical Thickness	50 to 10^5 Å	5% total thickness	0.1% of total thickness	Estimate made on slide to slide repeats
Optical Thickness/ layer	50 to 10^5 Å	50 to 100 Å	0.1% of layer thickness	Estimate of optical turning point accuracy
Optical Thickness Total	0.25 to 150 microns	50 to 100 Å (final layer)	0.1% of total thickness	Ending phase and thickness of final layer is critical
Substrate Temperature	40 to 350 °C	2-5 degrees	5 to 10 degrees uniformity	Temperature can strongly effect the sticking coefficients
Material Rates	0.2 to 30 Å/sec	<1 Å/sec	<.2 Å/sec	Crystal Oscillators—tooling factors required
Refractive Index	1.3 to 4.2	2%	<0.5%	Optical peak to valley amplitudes
Refractive Index Amplitude	.01 to .5	N/A	0.002	Not directly measurable using current techniques
Film Stress	0+/- $50x10^6$ kg/m^2	N/A	<1000 kg/m^2	Research capability only—no current commercial method
Index Distribution	< 2 %	N/A	<0.5%	Not insitu method, post characterization: 2%
Optical thickness Distribution	< 10%	N/A	<0.1%	Not insitu method, post characterization: 2%

Single point optical monitoring provides some feed back on optical properties, but has a number of limitations. These limitations include: poor sensitivity, monitoring at a single remote point and simplistic data processing schemes which are prone to errors. Single point optical monitors can not extract the optical properties needed to precisely control an index profile over very long periods of time. Broadband white light sources typically used in optical monitors do not provide adequate dynamic range for fabricating films of high optical density (OD). Table 2 provides estimates of the accuracy needed for the precise control of complex optical films.

Index Profile

In addition to selection of the materials, deposition methods, and monitors, a method of controlling the refractive index of the rugate profile must be determined. In come cases, the entire profile is determined prior to deposition and the 'prescription' simply followed. In most cases, though, closed loop control is necessary. For the multi-line sine wave rugate, the index profile is calculated as:

$$N_i = N_{ave} + \Sigma\, amp_j * \text{sine}\,(OT_j*4\pi/(\lambda_j * T_j) + \theta_j)\ [7]$$

Where profile variables are:

N_1	low index material
N_2	high index material
N_{ave}	average index
N_{sub}	substrate index
N_i	immediate index
OT_F	effective optical thickness for film
OT_j	optical thickness at each wavelength

λ_j = Rugate wavelength
Amp_j = Amplitude of index excursion for each line
θ_j = Starting phase of the index profile

Optical thickness is monitored on-band for each rugate wavelength or inferred from off-band measurements. The monitor determines when each rugate cycle has been completed and the controller adjusts the next cycle accordingly.

The index profile is generated by incrementing the film thickness and calculating the immediate index for the new film thickness. The average index is added to the summed index. The film thickness increment and the immediate index are passed to a characteristic matrix routine for calculation of performance.

An important point to consider is how the film increment is defined. The film increment can be a constant film thickness, or it can be a constant optical thickness. From the standpoint of modeling filter performance, the difference is immaterial—the answer is the same in either case. However, from the standpoint of modeling the process, the difference impacts monitor and source considerations. Constant optical thickness produces a smoothly varying sinusoidal response from the optical monitor. However, the incremental mechanical thickness of the film is changing. A constant increment physical thickness presents a constant material arrival rate, and this may be an important consideration for ion assisted processes.

Rate control of (at least) two materials of different refractive indices is required for co-evaporation to produce the desired composite index. Refractive index, n, is a function of the mixing ratios of the two materials. While several moodels have been used as a starting point in predicting composite refractive index[2], empirical data is usually required. The effective index is a function of relative rates, sticking coefficients and film density. For the purposes of this discussion, Bruggeman theory is used [10].

Constant Deposition Rate

For the case where constant combined rate is desired throughout the run,

Assume: $R_2 = R_1*(N_1^2-N_i^2)/(N_i^2-N_2^2)$and
: Rtotal = R1 +R2

Where: R_1 and R_2 are evaporation rates for materials with index N_1 and N_2

Then: $R_{total} = R_1(1+(N_1^2-N_i^2)/(N_i^2-N_2^2)\ )$

$R_1 = R_{total}\,/\ (1+(N_1^2-N_i^2)/(N_i^2-N_2^2)\ )$

Step 1: given Rtotal, and each index (N_1, N_2 and N_{ave}),

calculate: R_1,
$R_2 = R_{total}\ -R_1$

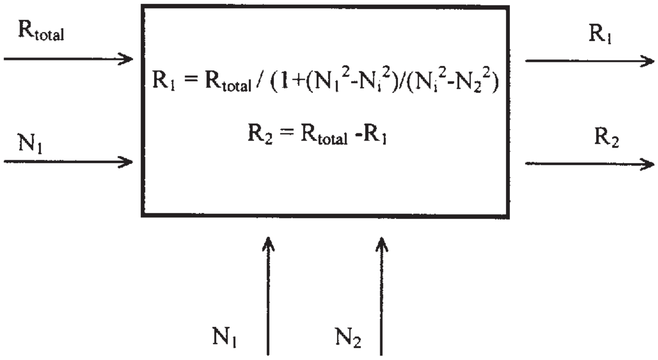

Figure 4. Data flow diagram illustrates the case where a constant total deposition rate is maintained during the run.

Constant Optical Thickness Rate

For the case where constant optical thickness rate is desired,

Assume: $R_2 = R_1*(N_1^2-N_i^2)/(N_i^2-N_2^2)$

$R_{total} = R_1 + R_2$

and: $\delta OT/\delta t = \text{constant} = N_{ave}*R_{total} = N_i*R_{t'}$

Then: $R_{t'} = R_{total}* N_{ave}/N_i$

$R_1 = R_{t'} / (1+(N_1^2-N_i^2)/(N_i^2-N_2^2))$

Step 1:given R_{total}, and each index (N_1, N_2 and N_{ave}),

calculate: R_1,

$R_2 = R_{total} - R_1$

assume constant Σ Rates

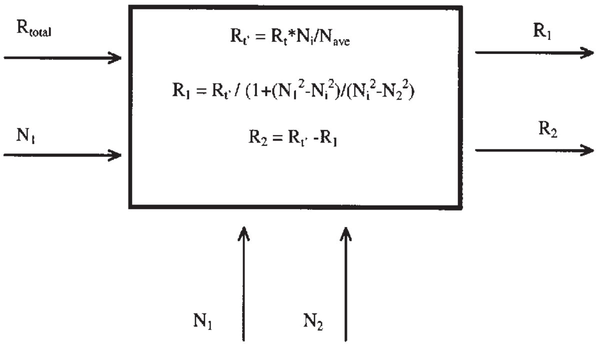

Figure 5. Data flow diagram illustrates the case where a constant optical thickness rate is maintained during the run.

Source Rates

Deposition rates are typically monitored at 10 Hz, and updated once per second. The film setpoints for a Rugate film may be updated every 5 seconds which is generally within the response capability of most types of sources. Rugate cycles or discrete layers complete every 1 to 5 minutes, and a unit of optical density is gained every 30 to 100 minutes. In the case of Rugate films, any systematic variation which affect the relative mixing ratio of the material blend, will produce unwanted, spurious reflection notches in the film. Examples of systematic variations include substrate rotation, source lead and lag, and undamped control oscillations from the source and temperature PID controllers. The process control is better if small incremental rate changes are made rather than large changes.

While excellent results have been demonstrated using electron -beam (e-beam) evaporation, a high level of process maintenance and operator supervision is required. An alternative to e-beam evaporation is magnetron sputtering. While this process exhibits typically lower deposition rates than thermal processes, it is much more stable. Power to sputter rate parameters are very repeatable and indicative of the status of the process. Good results using stoichiometric control of index have been demonstrated as well as co-deposition of two materials. Source aging is much less intrusive for magnetron sputtering than e-beam and resistive evaporation where significant changes in source plume distribution and material collapse can occur throughout the coating run.

IMPROVEMENTS IN PROCESS CAPABILITY

Control algorithms need to be sensitive to random and systematic process variability. Many process controllers are simple PID systems. These systems are prone to be over- or under damped. Improper adjustment of PID parameters can lead to the system being under responsive, or to ‘ringing’. Changes in process parameters such as source depletion, change the desired setpoints. The monitor system should be capable of detecting control driven parameters—ringing, long term drift, excessive power, high frequency noise. Understanding the source of error is needed to properly diagnoses and improved process yield.

Multiple resolution analysis of insitu sensor data using wavelet transforms provides the means of extracting both short term and long term trends from a common data stream. A method for monitoring the fabrication of discrete and Rugate filters using the Haar transform has been proposed [3]. This method shows promise for improved data analysis and storage, trend analysis, and deduction of waveform, dispersion, and systematic errors.

This technique begins by describing the average of the time series, and then successively resolves the time series into more detailed layers. The lowest resolution coefficients describe optical density growth and absorption. The more detailed layers describe systematic and periodic variations due to the growth of optical thickness. Separate analysis of data for different time regimes provides insight into different physical parameters. Least square fit to the low order terms relate to parameters such as film absorption and growth of optical density. Windowed Fourier transforms of periodic structure in the coefficients of the detailed layer provides insight into a number of performance parameters such as the period and amplitude of the optical thickness cycle which is characteristic of Rugate design.

Multipoint monitoring is necessary to monitor and control source plume and temperature uniformity. Monitors need to simulate actual substrate conditions; substrate temperature, type, cleanliness, and quality all affect the validity of a deposition measurement. Spectral flexibility of the sensors, i.e. the ability to easily adapt from the UV to the far IR, is necessary.

Reflectometry, photometry, ellipsometry, and interferometry, can all provide critical process data. Both the individual sources and the blend needs to be monitored. Using a combination of these techniques, optical thickness, optical thickness rate, refractive index, film stress, absorption, and distribution of optical thickness and refractive index can be determined. Sensor fusion, i.e., the ability to combine data from different sensors and different locations is key to cost effective production of broad band filters.

The feasibility and efficacy of producing and integrating small, fiber based multi-purpose sensors into the rugate fabrication process has been demonstrated [5].

SUMMARY

In designing a rugate process several considerations should be added to the many choices already facing the optical coating engineer for traditional coatings. Index profile generation should be chosen to best match both the monitoring scheme and the deposition process. It is also best not to rely on mixing ratio equations to predict required rates for given refractive indices. New algorithms for in process data analysis and trend analysis should be considered.

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