Sensitivity-directed refinement for designing broadband blocking filters

T. Amotchkina,1 U. Brauneck,2 A. Tikhonravov,1 and M. Trubetskov,1,3,*
1Research Computing Center, Moscow State University, Leninskie Gory, 119991, Moscow, Russia, 2Schott, Rue Galilee 2, CH-1401 Yverdon-les-Bains, Switzerland 1Max-Planck Institute of Quantum Optics, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Abstract: We developed a new method aimed at designing short-pass filters, long-pass filters and filters blocking sidebands of Fabry-Perot bandpasses. The method is an automated version of a non-straightforward empirical approach invented as a result of many years' experience in design and production of optical coatings. The method allows obtaining near-quarter-wave solutions in a few seconds. In many cases these solutions are more advantageous for deposition systems.

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References and links
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1. Introduction
Due to tremendous progress in thin film technology and growing demands on coating performances, the development of new design approaches is still in a focus of optical coating engineers. Along with general purpose design techniques such as refinement, needle optimization, gradual evolution [1–5], special approaches aimed at different types of
multilayer coatings are being actively developed. For example, specific methods for designing dispersive mirrors [6,7], minus and notch filters [8–11], WDM filters [12,13] have been implemented by different authors.

Very often, optical coating engineers in order to avoid complicated design solutions invent and use their own empirical approaches aimed at obtaining designs with some specific structures. Design preferences are often determined by technical requirements of deposition plants and monitoring systems in their disposal. In particular, for a wide range of filter design problems, quarter-wave stacks (QWS) or near-quarter-wave stacks (NQWS) solutions are more beneficial for the production.

NQWS do not contain thin layers. This represents an advantage in the case of deposition plants, that cannot produce layers thinner than 15 nm with a good uniformity because of a relatively low calotte rotation speed. For example, if the substrate holder rotates with the speed of about 30 rpm and the deposition rate is 0.3 nm/s, then the deposition of a 15 nm layer takes 50 sec or 25 rotations. Due to spatial non-uniformity of evaporated material flow and different positions of samples at the calotte, their layers may have different thicknesses. The deviation of layer thicknesses may reach 0.6 nm that is 4% of 15 nm layer. Therefore, in order to achieve good uniformity of about 1%, minimum 200 sec of deposition time or 100 rotations of the calotte are required.

In the case of the monochromatic optical monitoring, production yields of NQWS are higher, because large building blocks in such coatings can be monitored without changing the monitoring wavelength. Some real-life optical monitors (for example, Leybold OMS5000) use proven monitoring strategies that insure very good cut-off reliability for NQWS.

The new Sensitivity-Directed Refinement (SDR) method allows obtaining NQWS with excellent spectral performances. Using different settings of the method, it is possible to obtain not one but several design solutions. The method is highly appropriate for designing broadband blocking filters like short-pass, long-pass filters, or filters blocking sidebands of Fabry-Perot bandpasses. The robust version [14] of the SDR algorithm allows taking into account the requirement on stability of the design solutions to possible variations of the refractive indices as well as to errors in layer thicknesses.

In Section 2 the new SDR method is described in detail. In Section 3 the method is applied to three design problems. Final conclusions are presented in Section 4.

2. Description of the Sensitivity-Directed Refinement method

Denote the number of design layers as $m$, layer thicknesses as $d_1, \ldots, d_m$. Let $\hat{S}(\lambda_j)$ and $S(d_1, \ldots, d_m; \lambda_j)$ be target and actual spectral characteristics specified on the wavelength grid of interest $\{\lambda_j\}, j = 1, \ldots, L$; and $\Delta S_j$ – the tolerances. Deviations of actual spectral characteristics from the target ones are evaluated with the help of the merit function ($MF$):

$$MF(d_1, \ldots, d_m) = \left(\frac{1}{L} \sum_{j=1}^{L} \left[ \frac{S(d_1, \ldots, d_m; \lambda_j) - \hat{S}(\lambda_j)}{\Delta S_j} \right]^2 \right)^{1/2}.$$ (1)

Let $\delta_H$ and $\delta_L$ be levels of relative errors in high and low index layers, respectively. Then, a set of $m$ disturbed designs with layer thicknesses $d_1, \ldots, d_i(1+\delta_{H,L}), \ldots, d_m$, $i = 1, \ldots, m$ is defined. For each disturbed design merit function variations ($\Delta MF_i$) are evaluated and layer sensitivities ($LS_i$) are calculated as:

$$\Delta MF_i = \left| MF(d_1, \ldots, d_i(1+\delta_{H,L}), \ldots, d_m) - MF(d_1, \ldots, d_m) \right|, \quad LS_i = \frac{\Delta MF_i}{\max_{i=1,\ldots,m} \Delta MF_i} \times 100\%.$$ (2)
With the help of Eq. (2), all layers can be ranged with respect to their $LS$ values.

**Step 0.** A starting design is a combination of quarter-wave stacks with different wavelengths. The choice of a reasonable starting design can be usually done according to the positions of requested high reflection zones [1–3]. Designate starting layer thicknesses as $d_{F,1}, d_{F,2}, \ldots, d_{F,m}$. The letter “$F$” in the subscript denotes “Fixed” state of layer thicknesses.

**Step 1.** Layer sensitivities of all starting design layers are calculated and a layer with $LS = 100\%$ is to be found. Let $k_1$ be the number of this layer. The merit function is minimized with respect to the thickness of this most sensitive layer:

$$MF\left(d_{F,1}, \ldots, d_{F,k_1}, \ldots, d_{F,m}\right) \rightarrow \min$$  \hspace{1cm} (3)

In Eq. (3) the letter “$A$” in the subscript denotes “Active” state of the chosen layer. As a result of the optimization, an intermediate design is obtained.

**Step 2.** Layer sensitivities of all layers of the intermediate design obtained at the Step 1 are evaluated, and a layer with the maximum layer sensitivity among all layers except for the layer number $k_1$ is found. Let $k_2$ be the number of this layer. Note, that at this and next steps the found maximum $LS$ value is not necessary 100% because some layers have been already activated at the previous steps and have been excluded from considerations. Then, the merit function Eq. (1) is optimized with respect to the layer thicknesses with the numbers $k_1$ and $k_2$:

$$MF\left(d_{F,1}, \ldots, d_{A,k_1}, \ldots, d_{A,k_2}, \ldots, d_{F,m}\right) \rightarrow \min$$  \hspace{1cm} (4)

After minimization of the merit function given by Eq. (4), a new intermediate design is found. Minimization of the merit function can be performed by various methods, for example, Quasi-Newton, Newton or Sequential Quadratic Programming (SQP) [15,16]. The only constraints on layer thicknesses are conditions $d_i \geq 0$, yet if necessary additional requirements $\hat{d}_i \leq d_i \leq \tilde{d}_i$ can be introduced (simple bounds constraints).

**Further steps and termination.** These iterations continue further, the number of active layers is increased at each step, and the value of $MF$ is gradually decreased. The iterations are terminated when a desired spectral performance is achieved or all $m$ layers become active.

For the sake of convenience, only the simplest version of the SDR has been presented above. In this version the number of layers activated at each step is $p = 1$. In general, there are several algorithm parameters that can be controlled. First of all, at each step the method allows activating arbitrary number $p \geq 1$ of layers having maximum sensitivity values. Evidently, if all $m$ layers are activated at the very beginning, then the SDR becomes a standard refinement procedure. Secondly, after several optimization steps, the insertion of new layers with the help of the needle optimization technique is possible as an additional option. At a needle step, only active design layers are considered as possible places for needle insertions. Thirdly, the levels of errors $\delta_H$ and $\delta_L$ can be also used as parameters of SDR.

### 3. Numerical examples

3.1 **Example 1: designing a blocking filter**

Let target transmittance be less than 1% in the spectral ranges from 400 nm to 480 nm and 680 nm to 806 nm and more than 99% in the range from 557 nm to 587 nm, see Fig. 1(a). The merit function is calculated on the wavelength grid containing 656 points. For this and next design problems, OptiLayer Software was used [17].
In all examples, high and low index materials are Nb$_2$O$_5$ and SiO$_2$, respectively. Their refractive indices are described by Cauchy formula (the wavelength is expressed in nanometers):

$$n(\lambda) = A_0 + A_1 \left(\frac{1000}{\lambda^4}\right) + A_2 \left(\frac{1000}{\lambda^2}\right)^4$$

with $A_0 = 2.2185$, $A_1 = 0.0218$, $A_2 = 3.999 \cdot 10^{-3}$ for Nb$_2$O$_5$ and $A_0 = 1.4653$, $A_1 = 0$, $A_2 = 4.71 \cdot 10^{-4}$ for SiO$_2$. The substrate is glass B270.

Fig. 1. Target and actual transmittances of starting, SDR and refined designs (a); design structures: starting and SDR designs (b), starting and refined designs (c).

In order to explain the method clearly, the manual version of SDR is demonstrated first. A combination of two QWS is chosen as a starting design: the layers 1 through 26 have $1.75$ QWOT (quarter-wave optical thickness) and the layers 27 through 46 have $1.0$ QWOT; reference wavelength is $440$ nm. Transmittance of the starting design is shown in Fig. 1(a), starting $MF$ value is $11.6$.

At the Step 1, $LS$ for all design layers are calculated. The $LS = 100\%$ corresponds to $k_1 = 14$. After minimization of $MF$ (Eq. (3)) with respect to $d_{14}$, an intermediate design having $MF = 7.35$ is obtained. At the Step 2, $LS$ of all layers are calculated again and a layer with the maximum $LS$ value among all layers with exception of the layer number 14 is searched for. It turns out, that the layer 24 is the most sensitive one at this step ($k_2 = 24$).

After minimization of $MF$ Eq. (4) with respect to the thicknesses $d_{14}, d_{24}$, the second intermediate design is obtained and $MF$ is decreased to the value $3.67$. Further evolution of $MF$ values and numbers of active layers are presented in Table 1. It is seen from Table 1 that only 9 steps of SDR are necessary to achieve zero $MF$ value.

| Step | Numbers of active layers | $MF$ value |
|------|--------------------------|------------|
| 0    | -                        | 11.60      |
| 1    | 14                       | 7.35       |
| 2    | 14, 24                   | 3.67       |
| 3    | 14, 24, 42               | 2.81       |
| 4    | 14, 24, 42, 23           | 2.58       |
| 5    | 14, 24, 42, 23, 4        | 2.45       |
| 6    | 14, 24, 42, 23, 4, 39    | 1.53       |
| 7    | 14, 24, 42, 23, 4, 39, 22| 1.37       |
| 8    | 14, 24, 23, 4, 39, 22, 2 | 0.6        |
| 9    | 14, 24, 42, 23, 4, 39, 22, 2, 25 | 0.0       |
The final design structure is plotted in Fig. 1(b). Transmittance of the final design is shown in Fig. 1(a). As mentioned above, only nine layers of the starting design were modified by SDR, thicknesses of other 37 layers were kept unchanged.

For comparison, the same design problem was solved with the help of a standard refinement (SQP method). The structure of the obtained design is presented in Fig. 1(c). The refined design also provides zero $MF$ value and exhibits an excellent spectral performance Fig. 1(a). However, now not nine as before but all layer thicknesses have been varied that makes more difficult a choice of monochromatic monitoring strategy with a small number of different monitoring wavelengths.

3.2 Example 2: designing a short-pass filter

In this case target transmittance is more than 97% in the range from 400 nm to 480 nm and less than 1% in the range from 520 nm to 900 nm, see Fig. 2(a). Reference wavelength is 600 nm and 60-layer design consisting of two QWS is taken as a starting design. The layers 1 through 30 have 1.35 QWOT and the layers 31 through 60 have 1 QWOT. Transmittance of the starting design is shown in Fig. 2(a).

After application of the two versions of the SDR with $p = 2, \delta_H = 1, \delta_L = 2$ and with $p = 3, \delta_H = 1, \delta_L = 1$, two different 60-layer NQWS, SPF1 and SPF2, are obtained. Both designs exhibit excellent spectral performance, see Fig. 2(a). Their structures in QWOT are shown in Fig. 2(b) and Fig. 2(c). In the course of SDR, 26 layers were activated in SPF1 design and 27 layers in SPF2 design.

3.3 Example 3: Designing a long-pass filter

Target transmittance is less than 1% in the spectral range from 425 nm to 670 nm and more than 97% in the range from 725 nm to 1200 nm, see Fig. 3(a). The merit function is calculated on the wavelength grid containing 309 points.

Reference wavelength is 475 nm and a 51-layer design consisting of two QWS is taken as a starting design. The layers 1 through 26 have 1.28 QWOT and the layers 27 through 51 have 1 QWOT. Transmittance of the starting design is shown in Fig. 3(a).

After application of the two versions of the SDR with $p = 2, \delta_H = 1, \delta_L = 2$ and with $p = 3, \delta_H = 2, \delta_L = 1$, two different NQWS, LPF1 (51 layers) and LPF2 (49 layers), are obtained. It is seen from Fig. 3(a) that the both designs exhibit excellent spectral performance. Their structures in QWOT are shown in Fig. 3(b) and Fig. 3(c). In the course of two SDRs, 12 and 11 layers were activated.
Designs obtained by SDR algorithm can be practically monitored using the strategies presented in Table 2. We performed a series of simulations assuming monochromatic monitoring with the strategies specified in Table 2 and simulation parameters close to those considered in [18]. The SDR designs demonstrated high production yield during the simulations.

Table 2. Practical monitoring strategies for the considered designs

| Design  | Witness Chip 1 | Witness Chip 2 |
|---------|----------------|----------------|
|         | Wavelength, nm | Layers         |
| Blocking Filter | 625            | 1-18           |
|          | 615            | 19-46          |
| SPF1    | 415            | 1-2            |
|         | 428            | 3-30           |
| SPF2    | 523            | 1-6            |
|          | 510            | 7-30           |
| LPF1    | 390            | 1-2            |
|          | 410            | 3-23           |
| LPF2    | 470            | 1-7            |
|          | 430            | 8-23           |

4. Summary

The proposed SDR method takes into account important practical requirement of closeness of design layer thicknesses to layer thicknesses of quarter-wave stacks. The idea of the method is based on many years experience in the design and production of optical coatings. The automatic version of SDR provides a possibility to obtain a series of near-quarter-wave solutions for complicated design problems in a short time. The obtained solutions exhibit excellent spectral performances. SDR method demonstrates outstanding results in designing edge filters and blocking filters.

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