Designing Coatings in the Presence of Manufacturing Errors

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Abstract: A novel robust optimization algorithm is demonstrated, which attempts to account for expected coating errors. Monte Carlo simulations show the robust approach improves manufacturing yields relative to conventional optimization.

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1. Introduction

The science of thin film design has seen rapid advance in the past few decades, with the introduction of both general and application specific optimization methods (e.g. [1, 2]). For the most part, however, design algorithms have not explicitly considered the effects of manufacturing tolerances during the optimization itself, though work has been done on methods for analyzing a plurality of existing designs to determine the most manufacturable [3].

In this paper, we propose a novel optimization method that explicitly takes the possibility for layer errors into account, compromising nominal performance in order to improve robustness against layer perturbations. In theory, one could attempt to optimize a coating merit function which involves a full Monte Carlo simulation of manufacturing statistics. However, such an approach would be computationally infeasible for all but the simplest designs. Our approach is a *deterministic* method that explicitly considers the effects of manufacturing tolerances, while retaining the fast convergence properties inherent to a deterministic algorithm. The presented method is generic and can be applied to many problems that are solved through numerical simulations.

Through Monte Carlo simulations of manufacturing errors, we compare the performance of a proof of concept antireflection (AR) coating designed with our robust optimization to that of a conventionally optimized AR coating. We find that the robust algorithm produces an AR coating with a higher manufacturing yield when root mean square layer tolerances are above approximately 1 nm.

2. Method

Our approach to robust optimization probes the exact merit function in a bounded space of potential thickness errors. While this results in a much more computationally involved optimization, the result is more robust to significant perturbation as the full structure of the merit function is considered in a neighborhood around a nominal solution. Furthermore, the robustness is guaranteed to be equal or better than that obtained with nominal optimization, and in the case where it is equal, no sacrifice in nominal optimality will be made.

For the purposes of developing this algorithm, we model manufacturing errors as independent random sources of additive noise, since any known systematic errors, such as miscalibration, can be best addressed in the actual production. Therefore, we assume that when manufacturing a mirror with layer thicknesses given by $\mathbf{x}$, statistically independent additive implementation errors $\Delta\mathbf{x} \in \mathbb{R}^n$ may be introduced due to variation in the coating process, resulting in an actual thicknesses $\mathbf{x} + \Delta\mathbf{x}$. We assume a mean of zero and a variance on each layer that is motivated by actual manufacturing errors. Here, $\Delta\mathbf{x}$ resides within an uncertainty set $\mathcal{U} := \{\Delta\mathbf{x} \in \mathbb{R}^n \mid \|\Delta\mathbf{x}\|_2 \leq \Gamma\}$. Note that $\Gamma > 0$ is a scalar describing the size of perturbation against which the design needs to be protected. For this paper, we took the manufacturing uncertainty to be normally distributed with a standard deviation of $\sigma = 1$ nm. The *robust optimization method* seeks to minimize the worst case cost via

$$\min_{\mathbf{x}} \quad g(\mathbf{x}) \quad \equiv \quad \min_{\mathbf{x}} \quad \max_{\Delta\mathbf{x}\in\mathcal{U}} \quad f(\mathbf{x} + \Delta\mathbf{x}). \tag{1}$$

When implementing a certain design $\mathbf{x} = \hat{\mathbf{x}}$, the possible realization due to implementation errors $\Delta\mathbf{x} \in \mathcal{U}$ lies in the neighborhood set $\mathcal{N} := \{\mathbf{x} \mid \|\mathbf{x} - \hat{\mathbf{x}}\|_2 \leq \Gamma\}$. Therefore, $g(\hat{\mathbf{x}})$, is the maximum cost attained within $\mathcal{N}$. Let $\Delta\mathbf{x}^*$ be one of the worst implementation error at $\hat{\mathbf{x}}$, $\Delta\mathbf{x}^* = \arg\max_{\Delta\mathbf{x}\in\mathcal{U}} f(\hat{\mathbf{x}} + \Delta\mathbf{x})$. Then, $g(\hat{\mathbf{x}})$ is given by $f(\hat{\mathbf{x}} + \Delta\mathbf{x}^*)$.

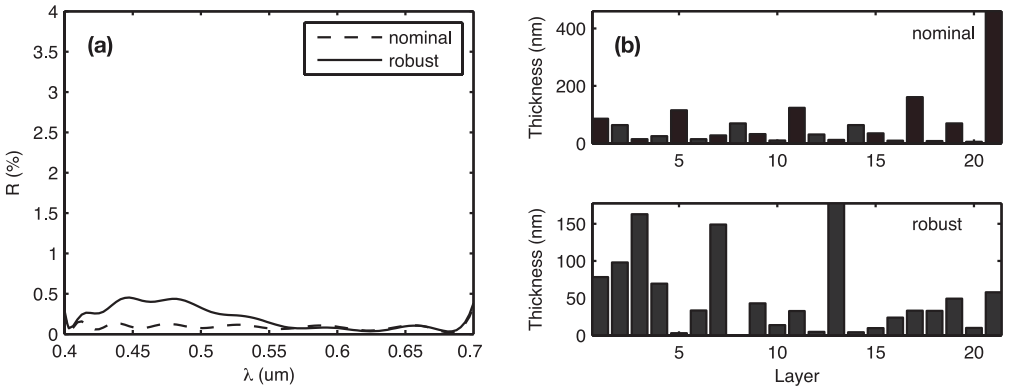

Fig. 1. (a) Reflectance of the nominally-optimized and robust-optimized AR coatings. (b) Layer thicknesses of nominally-optimized (top) and robust-optimized (bottom) designs.

Since we seek to navigate away from all the worst implementation errors, the inner maximization problem needs to be solved first. We conduct local gradient ascent searches to determine worst configurations within $\mathcal{N}$.

It is well known that the reflection coefficients of thin-film stacks are closely related to the Fourier transform of the layer thicknesses [5]. One promising class of "rare" perturbations to eliminate from consideration are thus those which have strong correlations between the layers. A straightforward way to do this is to restrict the search to the class of error vectors where all Fourier components have a uniform amplitude [6]. Therefore, for the inner maximization problem, we obtain the set of local maxima in the phase space using standard unconstrained gradient-based optimization.

Once worst-case neighbors are identified, a direction is sought along which an updated neighborhood would not include these worst-case scenarios any longer. This direction is a vector that spans the largest angle $\Theta \geq 90^\circ$ to all worst implementation errors at $\hat{\mathbf{x}}$ in the *set of worst implementation errors* $\mathcal{U}^*(\hat{\mathbf{x}}) = \arg\max_{\Delta\mathbf{x}\in\mathcal{U}} f(\hat{\mathbf{x}} + \Delta\mathbf{x})$. To navigate away from the elements in $\mathcal{U}^*(\hat{\mathbf{x}})$, a descent direction $\mathbf{d}^*$ can be found efficiently by solving the following second-order cone problem:

$$\begin{aligned} \underset{\mathbf{d},\beta}{\text{minimize}} \quad & \beta \\ \text{subject to} \quad & \|\mathbf{d}\|_2 \leq 1 \\ & \mathbf{d}\cdot\Delta\mathbf{x}^* \leq \beta \qquad \forall\Delta\mathbf{x}^* \in \mathcal{U}^*(\hat{\mathbf{x}}) \\ & \beta \leq -\epsilon, \end{aligned} \tag{2}$$

where ϵ is a small positive scalar, β is an auxiliary variable, and $||\cdot||_2$ is the Euclidean norm. A feasible solution to Problem (2), $\mathbf{d}^*$, forms the maximum possible angle $\theta_{\max}$ with all $\Delta\mathbf{x}^*$. This angle is always greater than 90° due to the constraint $\beta \leq -\epsilon < 0$. This constraint guarantees that d^* will provide an updated design neighborhood that excludes all known $\Delta\mathbf{x}^*$. When Problem (2) is infeasible, then $\hat{\mathbf{x}}$ is a robust local minimum. Reference [4] provides a detailed discussion on the actual implementation.

Finally, the algorithm concludes with a reoptimization of the robust solution using a standard nominal optimization, but with a very large termination tolerance so the stack is not perturbed enough to significantly affect the robustness. Since the nominal performance is not considered at all during the robust optimization, the nominal performance can often be significantly improved without much change in the worst-case cost.

3. Results

For a proof of concept, we designed an AR coating for the visible, with the merit function being simply the average reflectance, evenly weighted, from 400 nanometers to 700 nanometers. The material system was assumed to be Ti_2O_5/SiO_2 on a fused silica substrate, with full material dispersion considered. The number of layers was limited to 21, though the optical thickness was not limited.

To begin, a nearly optimal AR coating was designed with characteristics similar to those found in [7], using standard gradient descent techniques. The starting point was a trivial stack composed of uniform layers of roughly 1/8 wave optical thickness. This design, which we refer to as the nominally-optimized coating, has an average reflectance of around 0.1%. We then applied the robust algorithm, starting with a random perturbation of the same starting point (to avoid falling into a local minima close to our first design). As expected, the robust design has a significantly worse

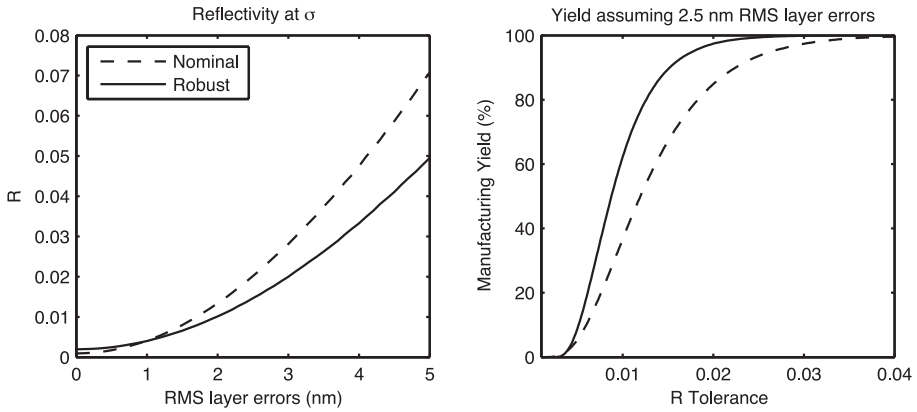

Fig. 2. Simulated performance of the nominal and robust designs in the presence of manufacturing errors: (a) reflectance at one standard deviation away from the mean for a range of layer tolerances; (b) manufacturing yield, assuming layer thickness errors of 2.5 nm RMS.

nominal performance, with an average reflectance of roughly 0.25%. The theoretical performance of the two designs are compared in Fig. 1. The significant increase in reflectance for the robust design in the absence of manufacturing defects is the unavoidable "Price of Robustness."

To assess the effects of statistical deposition errors, we performed Monte Carlo simulations assuming independent, normally distributed additive errors applied to each layer. The mean of the errors was assumed to be zero, with the Monte Carlo simulation repeated for a range of standard deviations from zero to 5 nanometers. Each Monte Carlo run involved 10^6 samples.

The reflectance of the manufactured distribution one sigma away from the mean is displayed in Fig. 2(a) for both designs. As expected, for low variance the nominal design is better. However, once layer errors progress beyond 1 nm, the robust design proves superior, with the expected manufacturing distribution of the nominally-optimized design growing faster with increasing layer errors.

In Fig. 2(b), we show the expected yield (i.e. the percentage of coatings which posses a minimum performance) for a range of target reflectivities, assuming an RMS layer variation of 2.5 nm. Despite being designed to have more than twice the reflectivity, the robust design yields significantly more than the nominal stack above a tolerance of about 0.2% average reflectance. While the difference in yield is never more than a factor of two, this would correspond to a 50% reduction in marginal unit production cost, a significant amount in that context.

4. Conclusions

Our robust optimization method explicitly seeks to minimize the worst-case performance. Fortunately, doing so evidently also improves the statistical performance, as demonstrated in Fig. 2. That this would be the case is not obvious, and it is fortuitous that a deterministic algorithm can yield improvement in statistical performance. A series of Monte Carlo simulations were performed with varying standard deviations at the robust and the nominal optimum. The spread of the distribution for the nominal optimum design increases rapidly beyond σ, while the robust optimum degrades more moderately. Further work is underway to determine how to best choose the ideal σ in the robust algorithm for a given statistical variance of layer errors.

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