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Optimized Ternary Coatings: Design and Performance

Innocenzo M. Pinto, Vincenzo Pierro

On behalf of the USannio/UniSA VCRD/OWG Group
Summary

• Relevance of Coating Noise
• Coating Model
• Coating Optimization
• Ternary Coatings
• Optimized aSi/Ta2O5/SiO2 Coatings
• Conclusions
Noise Budget in GW Detectors

[S. Waldman, LIGO-P0900115]

Visibility volume & event rate \( \propto PSD_{floor}^{3/2} \)

... a 5\(\mu m\) thick film sets the performance of a 5\(Km\) size detector!!
Coating Model

Coating T-matrix

\[ \mathbf{T} = \mathbf{T}_1 \cdot \mathbf{T}_2 \cdot \ldots \cdot \mathbf{T}_{N_T} \]

Single layer T-matrix (normal indicence)

\[ \mathbf{T}_m = \begin{bmatrix} \cos (\psi_m) & (i/n^{(m)}) \sin (\psi_m) \\ i n^{(m)} \sin (\psi_m) & \cos (\psi_m) \end{bmatrix} \]

Individual layer phase-thickness and complex index

\[ \psi_m = \frac{2\pi}{\lambda_0} n^{(m)} d_m, \quad n^{(m)} = n_r^{(m)} - i k^{(m)} \]

Coating reflection coefficient and effective index

\[ \Gamma_C = \frac{1 - n_C}{1 + n_C}, \quad n_C = \frac{T_{21} + n_s T_{22}}{T_{11} + n_s T_{12}} \]

Coating transmittance

\[ \tau_P = \frac{P_{\text{in}}}{P_+} = 1 - |\Gamma_C|^2 \]

Top and bottom face fields

\[ \begin{bmatrix} E^{(S)} \\ Z_0 H^{(S)} \end{bmatrix} = \mathbf{T}^{-1} \begin{bmatrix} E^{(0)} \\ Z_0 H^{(0)} \end{bmatrix}, \quad E^{(0)} = E_{\text{inc}} (1 + \Gamma_C) \quad Z_0 H^{(0)} = E_{\text{inc}} (1 - \Gamma_C) \]

Coating absorbance

\[ \alpha_P = \frac{(P_{\text{in}} - P_{\text{out}})}{P_+} \]

\[ P_{\text{in}} = \tau_P P_+ \quad P_+ = \frac{1}{2Z_0} |E_{\text{inc}}|^2 \quad P_{\text{out}} = \frac{1}{2} \text{Re}(E^{(S)} H^{(S)*}) \]

[I. Pinto et al., Ch. 12 in Optical Coatings and Thermal Noise in Precision Measurements, G. Harry et al, Eds, Cambridge Un. Press 2012]
Coating Model, contd.

\[ S_B(f) = \frac{2k_B T}{\pi^2 f} \frac{1 - \sigma^2}{w^2 Y} \phi_c \]

, where

\[ k_B = \text{Boltzmann constant} \]
\[ T = \text{absolute temperature} \]
\[ w = \text{beam waist} \]

\[ \phi_c = \sum_{m=1}^{N_T} d_m \eta_m \]

, where \( d_m = \text{thickness of m-th layer, and} \)

\( \eta_m \) is the specific loss angle (loss angle per unit thickness) of the material in layer-m.

If \( K \) different materials are used, the \( \eta_m \) (\( m = 1, 2, ..., K \)) can be inferred easily from direct measurement of coating thermal noise (PSD) on \( K \) (or more) coatings using the same \( K \) materials with different thicknesses [Principe et al, PRD-91 (2015) 022005].

Alternatively, the \( \eta_m \) can be related to the viscoelastic properties of the layers and the substrate, via a suitable application of the F-D theorem, yielding, e.g., the approximate formula

\[ \eta_m = \phi_m \left[ \frac{Y}{Y_m} \frac{(1 + \sigma_m)(1 - 2\sigma_m)}{(1 + \sigma_m)(1 - \sigma^2)} + \frac{Y_m}{Y} \frac{(1 + \sigma)(1 - 2\sigma^2)}{(1 - \sigma)(1 - \sigma_m^2)} \right] \]

where \( (\phi_m, Y_m, \sigma_m) \) are the mechanical loss angle, and the Young and Poisson moduli of the material in layer-m, and \( (Y, \sigma) \) those of the coating substrate.

[V.B. Braginsky et al., Ch. 3 in Optical Coatings and Thermal Noise in Precision Measurements, G. Harry et al, Eds, Cambridge Un. Press 2012]
Coating Optimization - Background

  brute-force robust genetic optimization based study of optimal thicknesses for minimum TN at
  prescribed $\tau_p$; reveals end-tweaked quasi-Bragg stacked doublets structure;

-Ogin et al. [LIGO-G0800204]
  port of USannio optimization code (originally in Wolfram-Mathematica©), to LIGO – BENCH;

-Principe et al., [LIGO-T080337; Optics Expr. 23 (2015) 10938]
  extension of $\tau_p$ constrained thickness optimization to the dichroic case;

-Villar et al. [LIGO-G0906647 ; LIGO-G090887 ; Phys. Rev. D81 (2010) 122001]
  direct TN measurement (@ Caltech TNI) on thickness optimized prototypes designed at USannio
  and deposited at LMA;

-Kondratiev et al. [LIGO-P1000145, Phys. Rev. D 84 (2011) 022001]
  improved TN model, and refined thickness optimization results;

-Pinto et al. [Ch. 12 in Optical Coatings and Thermal Noise in Precision Measurements, Cambridge
  Un. Press, 2012] – broad review of the subject, including Brownian, TO and PT noise;

-Morgado et al., [TN Workshop, Pisa, February 23th 2012]
  dichroic-optimized prototypes made at LMA (and used in aLIGO & adVirgo);

\/. 
Coating Optimization – Background, contd.

-Chalermsongsak et al., [LIGO-G1400040; LIGO-P1500054; Metrologia 53 (2016) 860]
  Thickness optimization of TO-noise dominated GaAs/AlGaAS coatings;

-Pierro et al., [LIGO-P2000457; Opt. Mater. 96 (2019) 109269]
  Pareto-front (tradeoff) based study of binary coating thickness optimization under $\tau_p$ and $\alpha_p$ constraints; confirms previous heuristics;

-Pinto, LIGO-G [LIGO-G2000218]
  TN minimization of stacked-triplet ternary coatings under $\tau_p$ and $\alpha_p$ constraints; comparison with optimized Bragg-doublet based ternary coatings à la Yam-Steinlechner;

-Pierro et al. [LIGO-G; LIGO-P2000519-v3; Exhaustive search of minimum-TN ternary QWL-layer coatings under $\tau_p$ and $\alpha_p$ constraints; confirms Steinlechner-Yam ansatz on structure of QWL ternary coatings;

-Pierro et al. [LIGO G21004209, LIGO-G2101040, this presentation; paper in preparation]
  Study of structure and performance of minimum-CTN ternary coatings, under $\tau_p$ and $\alpha_p$ constraints; with no a-priori assumption on morphology.

...
Coating Optimization – Formalization of Problem

Problem: find the coating design \( \{(d_m, M_m)|m = 1, 2, \ldots, N_T\} \) where \( M_m \) identifies the material in layer-\( m \) (from a given pool of material candidates), \( d_m \) is the thickness of layer-\( m \), and \( N_T \) is the number of layers, also to be determined, such that the coating transmittance and absorbance constraints are satisfied
\[
\tau_P \leq \tau_P^{(\text{max})}, \quad \alpha_P \leq \alpha_P^{(\text{max})}
\]
and the coating loss angle is minimal.

The above represents a typical constrained optimization problem where we seek a solution satisfying several conflicting requirements. Such problems are most conveniently handled by seeking the Pareto (or tradeoff) manifold of the problem.

Our Pareto manifold \( \mathcal{P} \) is a surface in the 3D space \((\tau_P, \alpha_P, \Phi_C)\) whose points correspond to the coating designs, \( \{(d_m, M_m)|m = 1, 2, \ldots\} \) for which the constraints are satisfied; these points represent different tradeoffs among the conflicting requirements, and \( \mathcal{P} \) provides a pictorial representations of how they relate. The strictly optimum design corresponds to the point of \( \mathcal{P} \) where \( \Phi_C \) is minimum.

Constructing the Pareto manifold \( \mathcal{P} \) is a nontrivial problem [S. Parisi et al., Neurocomputing 263 (2017) 3].
The BORG-MOEA Optimization Environment

Developed by D. Hadka and P. Reed at UPenn; freely available to Academic Users

http://borgmoea.org/

... the strength of BORG, compared to other similar/competing tools is that it attempts (and usually succeeds) in seeking adaptively the best evolutionary engine(s) to reconstruct the Pareto manifold as densely/closely as possible. This should be done adaptively, as the best choice depend on the structure of the manifold itself ...

Borg aliens appear in episodes of the Star Trek TV-serial. They are cyborgs, with both artificial and biological body parts, that evolve through a process of assimilation of different technologies and life-forms, aimed at perfecting their physical and mental power. Interestingly they have no individual will, sharing a single mind (the B-Queen).
Multi Material Coatings & MM Candidate Materials

Multimaterial Coatings

J. Steinlechner et al. [PRD91 (2015) 042001]; W. Yam et al. [PRD91 (2015) 042002].
Modify the simplest binary coating design consisting of alternating QWL layers of SiO2 and TiO2 :: Ta2O5, by using a denser but optically lossier material in the high-index layers closest to the substrate, where its higher optical absorption is irrelevant;

K. Craig et al. [PRL 122 (2019) 231102]
Discusses multimaterial coatings for ET;

MM candidate materials: aSi

J. Steinlechner et al. [PRL 120 (2018) 263602]
Discusses aSi based multimayerial coatings in detail;

L. Terkowsky et al. [PRR 2 (2020) 033308]
Discusses influence of deposition parameters on the optical absorption of aSi;

R. Birney et al. [PRL 121 (2018) 191101]
Discusses producing aSi with extremely low absorption;

S. Gras et al. [LIGO-G1901619]
Partially-oxidized aSi (SiO_x)

S.C. Tait et al. [PRL 125 (2020) 011102]
Realization and characterization of a ternary coating prototype using aSi;
MM candidate materials: $\text{SiN}_x$

H.-W. Pan et al., [PRD97 (2018) 022004]
   Structure and properties of PECVD SiNx on Silicon;
H.-W. Pan, Thesis [LIGO-P1900332]
   Extended discussion of PECVD SiNx technology;
J. Steinlechner et al., [PRD96 (2017) 022007]
   Data on extinction coefficient of SiNx at 1064 nm and at 1550 nm;
S. Chao et al. [LIGO-G1902341]
   Discusses extinction reduction in NH$_3$-free PECVD SiNx;
S. Chao et al. [LIGO-G]
   Discusses low-refractive-index silicon-oxynitrides.

More MM options

G. Vajente et al. [LIGO-2000296]
   Discusses several Germania dopings as well as Titania doped Silica.

Up-to-date Coating Materials Overviews

G. Vajente [LIGO-G1902056]
M. Granata et al., [Appl. Optics 59 (2020) A229]
Material Parameters

<table>
<thead>
<tr>
<th>Substrates</th>
<th>n</th>
<th>κ</th>
<th>ϕ</th>
<th>Y [Gpa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>aSi [a][b]</td>
<td>3.5@1550nm</td>
<td>1.22 10⁻⁵@1550nm</td>
<td>10⁻⁴@290K, 8·10⁻⁵@120K, 2·10⁻⁵@20K</td>
<td>147</td>
</tr>
<tr>
<td>SiNx [b][e][d]</td>
<td>2.28@1064nm</td>
<td>1.51 10⁻⁵@1550nm</td>
<td>8·10⁻⁵@290K, 2·10⁻⁵@120K, 1·10⁻⁵@20K</td>
<td>103.7</td>
</tr>
<tr>
<td>SiO₂ [e]</td>
<td>1.44 (all NIR)</td>
<td>8·10⁻⁸</td>
<td>5·10⁻⁵@290K, 1.7·10⁻⁴@120K, 7.8·10⁻⁴@20K</td>
<td>72</td>
</tr>
<tr>
<td>TiO₂::Ta₂O₅ [e]</td>
<td>2.05 (all NIR)</td>
<td>8·10⁻⁸</td>
<td>3.66·10⁻⁴@290K, interpolated@120K, 8.6·10⁻⁴@20K</td>
<td>140</td>
</tr>
</tbody>
</table>

Substrates: Silica @ 1064nm (n = 1.44; Y = 72 Gpa); cSilicon @ 1550nm (n = 3.58; Y = 160 Gpa [f],)

aSi, Ti::Ta$_2$O$_5$, SiO$_2$ based coating @ 20K
\[ \kappa_{aSi} = 10^{-5} \]
Structure of Optimal Solution

Yielding minimal \( \phi_C \) (minimal thermal noise) under the constraints

\[
T = 20K, \kappa_{aSi} = 10^{-5}
\]

\[\tau_P \leq 6\text{ppm} \quad \alpha_P \leq 1\text{ppm}\]

CTN PSD Reduction Factor: 0.0843614

The optimal design is *quite readable* ...
Best Tradeoff Solution: Absorption Distribution

Graph showing normalized absorption versus layer number for different materials: aSi, Ta₂O₅, and SiO₂. The graph includes an inset showing the optical thickness and CTN PSD reduction factor.

I.M. Pinto – Optimized Ternary Coatings - KIW8 (2021)
Best Tradeoff Solution, Spectral Response etc.

\[
\frac{\text{arg}[\Gamma]}{\pi} = 0.9988
\]

6ppm
Empirical distributions (histograms) of coating CTN-PSD reduction factor (w.r.t. current aLIGO/adVirgo design), transmittance and absorbance, for a sample of 5000 realizations featuring i.i.d. random - uniform thickness errors within ±1 nm in each layer.
... What if: **10x Larger** $\alpha$Si Extinction Coefficient?

\[ T = 20K, \ k_{\alpha Si} = 10^{-4}; \ cSi \text{ substrate} \]

CTN PSD Reduction Factor: 0.126505

... design is different (8 triplets + 5 doublets, different tapering); performance still very good (noise PSD reduction factor 0.126 instead of 0.084) ...
The original ternary designs proposed by Yam et al. and Steinlechner et al. consisted of QWL layers forming two stacks: one based on SiO$_2$/Ti::Ta$_2$O$_5$ (top stack); the other based on SiO$_2$/aSi (bottom stack), closest to the substrate, where the field (and hence the power loss) is weaker.

The optimization of such a design (number of doublets ($N_{\text{top}}, N_{\text{bot}}$) in the top/bottom stacks) has been investigated exhaustively in [Pierro et al., PRR 3 (2021), 023172], where step-by-step generalizations were also discussed. These include, in order of increasing complexity,

$>>$ non-QWL Bragg doublets in both the top and Bottom stacks;

$>>$ non-QWL, non-Bragg doublets in both the top and bottom stacks.

The plot below provides a comparison, at different temperatures, and different level of the optical extinction coefficient of the 2nd material, between the optimal ternary design and the optimized design à la Yam-Steinlechner.
Conclusions

- The minimum-CTN ternary coatings under prescribed upper bounds for transmittance and absorbance have been sought using a 2\textsuperscript{nd} generation (adaptive) evolutionary algorithm (the BORG-MOEA).

- For the special relevant case of aSi|Tantala|Silica coatings, the optimal coatings have a nicely readable structure, consisting of a stack of quasi-Bragg Larruquert-triplets, with a smooth (nearly parabolic) thickness tapering, on top of a stack of aSi|Silica doublets (with negligible thickness tapering). Optimal SiNx|Tantala|Silica coatings are similar.

- The optimal design features some extra reflectance on the 2\textsuperscript{nd} harmonic (useful for alignment), and zero E-field in the face; and is nicely robust against deposition errors.

- Compared to present aLIGO/adVirgo coatings, aSi based optimized ternary coatings yield CTN PSD reductions by a factor \( \sim 10 \) @ 20K, already at \( \kappa_{aSi} \sim 10^{-4} \) (achieved).

- This is on a par with the promise of crystalline coatings, with substantially milder technological challenges (and costs).
Thank you for your attention

ご清聴ありがとうございました

 관심을 가져 주셔서 감사합니다