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A General Formula for the Thermorefractive Noise Coefficient of Stacked-Doublet Mirror Coatings

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1. Purpose and Motivation

Thermoelastic and thermorefractive noise in highly reflective coatings for advanced interferometric gravitational wave detectors, induced by coating temperature fluctuations of both thermodynamic and photo-thermal origin (laser shot noise) have been the subject of intense recent research. This report is focused on the extension (and validation) of a formula originally proposed by V.B. Braginsly and co-Workers for the thermorefractive coefficient of highly reflective coatings consisting of N_d identical stacked low-high index doublets.

2. Coating Thermorefractive Coefficient

The temperature dependence of the refraction index of the coating materials affects the phase of the coating reflection coefficient. To first order in the temperature change ΔT , assumed uniform across the coating thickness, the resulting phase-shift is equivalent to an effective displacement Δx of the test-mass (coated-mirror) front-face with respect to its center of mass. This is readily seen from the formula yielding the change in the reflection coefficient following a shift Δx in the reference plane:

$$\Gamma(\Delta x) = \Gamma(0) \exp\left(i\frac{4\pi}{\lambda_0}\Delta x\right),\tag{1}$$

with λ_0 being the laser-source wavelength in vacuum. Here, and henceforth, a normally-incident time-harmonic $(\exp(\iota\omega t))$ plane-wave excitation is assumed. The coating effective thermorefractive coefficient β_{eff} is accordingly defined as follows:

$$\Delta x = \lambda_0 \beta_{eff} \Delta T . \tag{2}$$

An explicit expression for β_{eff} was first obtained in [1], for the special case of coatings made of cascaded quarter-wavelength (QWL) low-high index doublets, and is:

$$\beta_{eff} = \frac{n_H^2 \beta_L + n_L^2 \beta_H}{4(n_L^2 - n_H^2)},$$
(3)

where $n_{L,H}$ is the refraction index and $\beta_{L,H} = dn_{L,H} / dT$ the thermorefractive coefficient of the low and high index material, at the reference temperature $T = T^{(0)}$. Equation (3) was derived in [1] in the limit where the coating consists of an infinite number of QWL doublets.

In a subsequent paper [2] by the same Authors on related topics, it was mentioned, without further details, that equation (3) ought to be corrected as follows:

$$\beta_{eff} = \frac{n_L n_H \left(\beta_L + \beta_H\right)}{4\left(n_L^2 - n_H^2\right)}.$$
(4)

For the SiO₂ -Ta₂O₅ coatings presently in use in LIGO, Eqs. (3) and (4) predict comparable values for β_{eff} (-2.19·10⁻⁵ K^{-1} against -2.59·10⁻⁵ K^{-1}). On the other hand, they give markedly different results for increasing values of the ratio n_H / n_L and fixed $\beta_{L,H}$. In particular, Eq. (4) predicts a vanishingly small value for β_{eff} in the limit $n_H / n_L \rightarrow \infty$, which is counter-intuitive.

3. Generalization of Equation (3) to non-QWL Stacked Doublet Coatings

In this section we shall extend the approach for computing the coating thermorefractive coefficient formulated in [1] for QWL coatings, to the more general case of coatings consisting of identical cascaded doublets with arbitrary thicknesses.

Let $\Delta \overline{Y}_{in}$ the change in the input wave admittance (normalized to the vacuum one, $Y_0 = 1/Z_0$) caused by the thermorefractive effect due to a (uniform) temperature change ΔT in the coating. The coating reflection coefficient can be written:

$$\Gamma = \frac{1 - \overline{Y}_{in}}{1 + \overline{Y}_{in}} = \frac{1 - \overline{Y}_{in}^{(0)} - \Delta \overline{Y}_{in}}{1 + \overline{Y}_{in}^{(0)} + \Delta \overline{Y}_{in}} \approx \Gamma^{(0)} \left(1 - \frac{2\Delta \overline{Y}_{in}}{1 - \left(\overline{Y}_{in}^{(0)}\right)^2} \right), \tag{5}$$

where $\overline{Y}_{in}^{(0)}$ is the nominal $(T = T^{(0)})$ normalized coating input admittance, and the approximation is valid for $\Delta \overline{Y}_{in} \ll \overline{Y}_{in}^{(0)}$. Comparing the reflection coefficient in (5) to Eq. (1), expanded to first order in the shift Δx of the reference plane,

$$\Gamma(\Delta x) \simeq \Gamma(0) \left(1 + \iota \frac{4\pi}{\lambda_0} \Delta x \right), \tag{6}$$

and recalling the definition of β_{eff} in Eq. (2), we obtain

$$\beta_{eff} \approx -\frac{1}{2\pi i} \frac{\left(\Delta \overline{Y}_{in} / \Delta T\right)}{1 - \left(\overline{Y}_{in}^{(0)}\right)^2}.$$
(7)

Assume now the coating as being composed of N_d cascaded identical doublets, and let

$$\begin{pmatrix} E_{in} \\ Z_0 H_{in} \end{pmatrix} = \begin{pmatrix} \Theta_{11} & \Theta_{12} \\ \Theta_{21} & \Theta_{22} \end{pmatrix} \begin{pmatrix} E_{out} \\ Z_0 H_{out} \end{pmatrix}$$
(8)

the equation defining the inverse transmission matrix $\underline{\Theta}$ for a *single* doublet, where (E_{in}, H_{in}) and (E_{out}, H_{out}) are the electric and magnetic fields at the input and output terminal-planes of the doublet. In order to compute the coating input admittance $\overline{Y}_{in} = \overline{Y}_{in}^{(0)} + \Delta \overline{Y}_{in}$ we follow [1] in noting that for *high-reflectivity* coatings, such as those of LIGO, N_d will be very *large*, and accordingly one can make the *ansatz* that addition of a *single* further doublet *does not* change the coating input admittance. Hence, for the added doublet,

$$\frac{Z_0 H_{in}}{E_{in}} = \frac{Z_0 H_{out}}{E_{out}} = \overline{Y}_{in} , \qquad (9)$$

which, can be combined with (8) and solved for $\overline{Y}_{in} = \overline{Y}_{in}^{(0)} + \Delta \overline{Y}_{in}$. After expanding the transmission matrix to first order in ΔT we obtain $\Theta_{ij} = \Theta_{ij}^{(0)} + \Delta \Theta_{ij}$, i, j = 1, 2, whence, from (9):

$$\Theta_{12}^{(0)} \left(\bar{Y}_{in}^{(0)} \right)^2 + \left(\Theta_{11}^{(0)} - \Theta_{22}^{(0)} \right) \bar{Y}_{in}^{(0)} + \Theta_{21}^{(0)} = 0 , \qquad (10)$$

and

$$\Delta \overline{Y}_{in} = \frac{\Delta \Theta_{21} + \overline{Y}_{in}^{(0)} \left(\Delta \Theta_{22} - \Delta \Theta_{11}\right) - \left(\overline{Y}_{in}^{(0)}\right)^2 \Delta \Theta_{12}}{\Theta_{11}^{(0)} - \Theta_{22}^{(0)} + 2\overline{Y}_{in}^{(0)} \Theta_{12}^{(0)}}.$$
(11)

Note that equation (10) has two roots. The only one satisfying the physical requirement of vanishing in the QWL limit is:

$$\overline{Y}_{in}^{(0)} = \frac{-\left(\Theta_{11}^{(0)} - \Theta_{22}^{(0)}\right) + \sqrt{\left(\Theta_{11}^{(0)} - \Theta_{22}^{(0)}\right)^2 + 4\Theta_{12}^{(0)}\Theta_{21}^{(0)}}}{2\Theta_{12}^{(0)}}.$$
(12)

Equations (7), (11) and (12) provide the anticipated generalization of Eq. (3) to the more general case of coatings consisting of cascaded identical doublets with arbitrary thicknesses.

4. Validation of Equation (3) via Alternative Derivation

In order to solve the dilemma between eqs. (3) and (4) we propose an alternative derivation of β_{eff} . One can prove by complete induction that, to first order in ΔT , the inverse transmission matrix (8) of a coating consisting of N_d identical cascaded QWL doublets is given by:

$$\Theta_{11} = \left(-\frac{n_{H}^{(0)}}{n_{L}^{(0)}} \right)^{N_{d}} \left[1 + \frac{2N_{d}}{\pi} \left(\Delta \psi_{H} - \Delta \psi_{L} \right) \right],$$

$$\Theta_{12} = -\iota \left(\frac{\Delta \psi_{H}}{n_{L}^{(0)}} + \frac{\Delta \psi_{L}}{n_{H}^{(0)}} \right) S(N_{d}),$$

$$\Theta_{21} = -\iota \left(n_{L}^{(0)} \Delta \psi_{H} + n_{H}^{(0)} \Delta \psi_{L} \right) S(N_{d}),$$

$$\Theta_{22} = \left(-\frac{n_{L}^{(0)}}{n_{H}^{(0)}} \right)^{N_{d}} \left[1 - \frac{2N_{d}}{\pi} \left(\Delta \psi_{H} - \Delta \psi_{L} \right) \right],$$
(13)

where (see Eq. (A2) in the Appendix)

$$\Delta \psi_{L,H} = \frac{\pi}{2} \frac{\beta_{L,H}}{n_{L,H}^{(0)}} \Delta T, \qquad (14)$$

and

$$S(N_d) = \begin{cases} \sum_{m=-P}^{P} \left(\frac{n_L^{(0)}}{n_H^{(0)}}\right)^{2m}, & N_d = 2P + 1\\ -\sum_{m=-P}^{P-1} \left(\frac{n_L^{(0)}}{n_H^{(0)}}\right)^{2m+1}, & N_d = 2P \end{cases}$$
(15)

The coating is assumed as being terminated in a half-space with refraction index n_s . Hence, $E_{out} = n_s^{-1} Z_0 H_{out}$. This can be used in Eq. (8) to obtain the coating input admittance as:

$$\begin{split} \overline{Y}_{in} &= \overline{Y}_{in}^{(0)} + \Delta \overline{Y}_{in} = \frac{Z_0 H_{in}}{E_{in}} = \frac{\Theta_{21} + n_S \Theta_{22}}{\Theta_{11} + n_S \Theta_{12}} = \\ &= n_S \left(\frac{n_L^{(0)}}{n_H^{(0)}} \right)^{2N_d} \left[1 - \frac{4N_d}{\pi} \left(\Delta \psi_H - \Delta \psi_L \right) \right] \\ &- \iota \frac{\left(n_L^{(0)} \right)^2 n_H^{(0)} \Delta \psi_H + \left(n_H^{(0)} \right)^2 n_L^{(0)} \Delta \psi_L}{\left(n_L^{(0)} \right)^2 - \left(n_H^{(0)} \right)^2} \\ &+ \iota \left(\frac{n_L^{(0)}}{n_H^{(0)}} \right)^{2N_d} \frac{\left[\left(n_L^{(0)} \right)^2 + n_S^2 \right] n_H^{(0)} \Delta \psi_H + \left[\left(n_H^{(0)} \right)^2 + n_S^2 \right] n_L^{(0)} \Delta \psi_L}{\left(n_L^{(0)} \right)^2 - \left(n_H^{(0)} \right)^2} \\ &- \iota \left(\frac{n_L^{(0)}}{n_H^{(0)}} \right)^{4N_d} \frac{n_S^2 \left(n_H^{(0)} \Delta \psi_H + n_L^{(0)} \Delta \psi_L \right)}{\left(n_L^{(0)} \right)^2 - \left(n_H^{(0)} \right)^2} . \end{split}$$
(16)

All terms on the r.h.s of (16) vanish in the limit as $N_d \rightarrow \infty$, in view of the fact that $n_H^{(0)} > n_L^{(0)}$, except the second one, which gives back Eq. (3), in view of Eqs. (14) and (7). We are accordingly led to conclude that eq. (3) is not flawed, and should be accordingly used instead of (4). Note that in some releases of BENCH [3] Eq. (4) has been used instead of (3).

5. Minimizing β_{eff} - Optimum Coating Designs

A number of alternative stacked - doublets designs yielding the same power transmittance $\tau \approx 1 \, ppm$ are displayed in Figure 1, in terms of the number of doublets N_d , and the quantity ξ (which parameterizes the departure from the QWL design) defined in the figure inset. The corresponding values of $|\beta_{eff}|$ are shown in Figure 2, together with the partial contributions of the low (Silica) and high (Tantala) index layers, for the special case of SiO₂/Ta₂O₅ based coatings, as a function of the number of doublets N_d (the corresponding value of ξ can be deduced from Fig. 1). A broad but distinct minimum of $|\beta_{eff}|$ is observed as the number of doublets N_d is increased, resulting from the competing reduction/increase in the noise contribution from the Tantala/Silica. Remarkably, the optimal design turns out to be closest to the one minimizing the Brownian noise term [5].

6. Conclusions

From the above results, the following conclusions can be drawn: *i*) Eq. (3) should be used in place of Eq. (4); *ii*) the traditional QWL coating design does not yield the coating lowest thermorefractive coefficient – indeed, as shown in [4], the stacked-doublet coating design yielding the minimum total noise (including the Brownian, thermoelastic and thermorefractive terms) is distinctly different from the QWL; *iii*) a general formula, which includes (3) as a particular case, has been obtained for the thermorefractive coefficient of stacked-doublet coating with general thicknesses.

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References

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[3] R.E. Collin, *Foundations for Microwave Engineering*, Wiley-IEEE Press, NY, ISBN: 978-0-7803-6031-0 (2001).

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[5] G. Castaldi et al., LIGO-G070309-00-Z

Appendix - Single Doublet Transmission Matrix

The single-doublet inverse transmission matrix $\underline{\Theta}$ in Eq. (8) has the following elements:

$$\Theta_{11} = \cos \psi_H \cos \psi_L - (n_H / n_L)^{-1} \sin \psi_H \sin \psi_L$$

$$\Theta_{12} = \iota \left(n_H^{-1} \sin \psi_H \cos \psi_L + n_L^{-1} \sin \psi_L \cos \psi_H \right)$$

$$\Theta_{21} = \iota \left(n_H \sin \psi_H \cos \psi_L + n_L \sin \psi_L \cos \psi_H \right)$$

$$\Theta_{22} = \cos \psi_H \cos \psi_L - (n_L / n_H) \sin \psi_H \sin \psi_L$$

(A1)

where $\psi_{L,H} = \frac{2\pi}{\lambda_0} n_{L,H} d_{L,H}$ is the phase-thickness of the low/high index layers, $n_{L,H}$ and $d_{L,H}$ being the pertinent refraction index and (physical) thickness. To first order in the temperature fluctuation ΔT , one has:

$$n_{L,H} \simeq n_{L,H}^{(0)} + \beta_{L,H} \Delta T, \quad d_{L,H} \simeq d_{L,H}^{(0)} \left(1 + \alpha_{L,H} \Delta T\right),$$

$$\psi_{L,H} \simeq \frac{2\pi}{\lambda_0} n_{L,H}^{(0)} d_{L,H}^{(0)} \left[1 + \left(\frac{\beta_{L,H}}{n_{L,H}^{(0)}} + \alpha_{L,H}\right) \Delta T\right] \triangleq \psi_{L,H}^{(0)} + \Delta \psi_{L,H}$$
(A2)

where a superfix ⁽⁰⁾ denotes the reference $(T = T^{(0)})$ values, and $\beta_{L,H}$, $\alpha_{L,H}$ are the thermorefractive and thermoelastic coefficients of the (bulk) low/high index material at $T = T^{(0)}$. The focus here is on the thermorefractive effect, and the $\alpha_{L,H}$ term in (A2) is accordingly dropped.



Fig. 1 – Alternative designs of stacked doublet coatings based on SiO₂ ($n_L^{(0)} = 1.45$) and Ta₂O₅ ($n_H^{(0)} = 2.0654$) yielding the same power transmittance (0.9727 *ppm*) as the QWL design ($N_d = 21$) getting closest to *1 ppm*.



Fig. 2 - Thermorefractive coefficient values for the alternative 0.9727 *ppm* stacked – doublet designs shown in Figure 1 (black markers). Partial contribution of Silica (blue markers) and Tantala (red markers) also shown. $\lambda_0 = 1064 \text{ nm}$.