

Simulation-based Optimization of Detector Layer Thickness to Reduce Contamination-induced Etaloning

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ABSTRACT

Detector etaloning, caused by interference effects from multiple internal reflections within detector layers and from reflections on the detector backside, can significantly affect the spectral and radiometric performance of spectrally resolving instruments. In this work, the phenomenon is investigated in the context of space applications. The detector design aims to suppress etaloning to a level where dedicated correction procedures are generally unnecessary. However, contamination layers formed by spacecraft outgassing can modify the optical stack during flight and induce interference effects that were absent during ground calibration. Such contamination-induced etaloning may require in-flight mitigation strategies, including recalibration, post-processing correction, or thermal decontamination of the detector. Although previous studies have investigated the influence of individual contaminants, a systematic assessment of different contamination materials and strategies to reduce their impact through detector design optimization remains limited. This paper investigates contamination-induced etaloning in a representative backside-illuminated (BI) charge-coupled device (CCD) and presents an optimization approach for reducing sensitivity to contamination-induced etaloning. A thin-film modelling framework based on the Python Optical Coating Analysis Library (POCAL) is used to simulate transmission spectra for various detector architectures. Two representative mission scenarios are considered: a broadband imaging application (550–900 nm) and a medium-band imaging application (660–680 nm). The effects of Water, Water Ice, Siloxane, glues RTV615 and Loctite 3526, Hydrocarbon, and Carbon contamination layers are analyzed over a wide range of thicknesses. An optimization algorithm is developed to identify native oxide and anti-reflection coating thicknesses that minimize contamination-induced changes in the transmission spectrum while maintaining high transmission performance. For the broadband scenario, the maximum Root Mean Square Error (RMSE) is reduced by up to 18%, while the medium-band scenario achieves reductions of up to 29%. In addition, the transmission stability is improved for multiple contaminants. The results demonstrate that incorporating contamination effects during detector design can substantially reduce contamination-induced etaloning, improve transmission stability, and decrease contamination-related measurement errors in future space missions.

Keywords: BI-CCD, CMOS, contamination-induced etaloning, detector contamination, detector optimization, optical system optimization, spacecraft outgassing, thin-film modelling, transmission spectra

1. INTRODUCTION

Optical detectors consist of multiple layers with different thicknesses and material properties. The structure can be compared to a Fabry-Pérot etalon, where an optical medium lays within two highly reflective surfaces. The incident light gets reflected multiple times, leading to interference fringes, which is known as detector etalon [1].

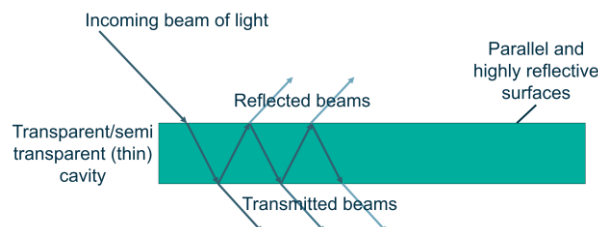


Figure 1: Typical Fabry-Pérot etalon configuration [1]

Depending on the detector design, fringes occur in different wavelength ranges. This effect has already been studied and methods to suppress etalon are known as well but come with a trade-off on quantum efficiency or mission costs. Thus, reducing the impact of detector etalon through postprocessing and calibration is widely applied [2]. This approach depends strongly on the assumption that the detector etalon will not change significantly during the mission lifetime. But especially when the detector has to be cooled down to cryogenic temperatures, various spacecraft materials that outgas can contaminate the detector surface [3]. In [4], it is shown that the contamination of a thin SiO₂ layer by water ice significantly alters both the amplitude and phase of the etalon fringes. Depending on the contaminants thickness, an entire fringe shift can be observed. Consequently, calibration data obtained on the ground may no longer accurately represent the in-flight detector response. As risk reduction, periodic detector decontamination through controlled heating can be implemented. This proven approach enables the removal of accumulated contaminants, helping to maintain detector performance throughout the mission lifetime [5]. In [6], where the impact of water ice contamination on the Euclid mission is examined, it is stated that the process of warming up, cooling down and recalibration lasts about a month, during which scientific observations are interrupted.

While previous studies have investigated the impact of specific contaminants, such as water ice, on detector etaloning, a broader assessment of different spacecraft outgassing products and strategies to reduce their impact through detector design optimization remains limited. This paper investigates the impact of spacecraft outgassing products on detector etaloning and explores how these effects can be mitigated through optimization of detector layer thicknesses. A thin-film modelling approach is employed, using the Python Optical Coating Analysis Library (POCAL) [7], to analyze the influence of contamination layers on detector transmission characteristics and etaloning behavior. The detector design presented in [2] is used to validate the thin-film modelling approach by comparing the simulated reflection, absorption, and transmission spectra obtained with POCAL to those reported in the reference.

A representative backside-illuminated CCD (BI-CCD) model is introduced. Two example missions are used to investigate the impact of contamination-induced etaloning in broadband and medium-band imaging scenarios. Various contamination materials and layer thicknesses are simulated, and their influence on the etaloning behavior is analyzed. Subsequently, an optimization approach is presented to identify detector layer thickness configurations that minimize the impact of contamination layers on etaloning.

2. METHODOLOGY

Simulation Framework

This study investigates the impact of contamination layers on detector etaloning using a thin-film modelling approach. The optical response of contaminated detector structures is simulated by calculating the wavelength-dependent transmission of multilayer stacks. The model is subsequently used to analyze the influence of different contamination materials and thicknesses on detector etaloning and to identify detector layer configurations that minimize contamination-induced fringe variations.

The optical simulations are performed using the Python Optical Coating Analysis Library (POCAL). POCAL implements the transfer matrix method to calculate the propagation of light through multilayer thin-film structures and determine their reflection, absorption, and transmission characteristics [7]. Its material library can be easily extended with contamination and detector materials. Additionally, the straightforward approach of defining the multilayer stack by stating the material and thickness of each layer in the order of the light incidence, simplifies the simulation of the transmission through the different contaminants or detector layers. To validate the modelling approach, the detector design presented in [2] is reproduced with POCAL. The simulated reflection, absorption, and transmission spectra are compared with those reported in the reference. Good agreement between the published and simulated results confirms the suitability of the model for investigating contamination-induced etaloning effects.

The optical modelling is subject to uncertainties arising from both the limited availability of detailed information on the detector architecture, such as the exact layer thicknesses, and the variability of wavelength-dependent refractive index and extinction coefficient data reported in the literature for the investigated materials. However, since this work focuses on demonstrating the influence of contamination layers on etaloning and on identifying layer thickness configurations that reduce this effect, small inaccuracies in these parameters do not compromise the overall conclusions, as the underlying mechanisms and trends remain unchanged. To investigate contamination-induced etaloning despite these uncertainties, a representative backside-illuminated CCD (BI-CCD) model is introduced, which serves as a simplification of the BI-CCD

designs. The model consists of a Silicon bulk as the photosensitive region, a native oxide layer of SiO_2 and an anti-reflective (AR) coating made of HfO_2 . As incident photons must reach and be absorbed within the photosensitive region to generate electron-hole pairs, the transmission into the silicon substrate is evaluated as the relevant metric for detector performance. The multilayer structure that is applied in this study is shown in Figure 2 including the contamination layer on top of the AR coating.

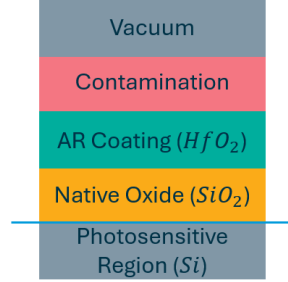


Figure 2: Multilayer structure of the representative BI-CCD model used for the contamination simulations. The model comprises the photosensitive region, SiO_2 layer, HfO_2 anti-reflection coating, and the contamination layer exposed to vacuum.

Two representative BI-CCD detector applications are used to investigate contamination-induced etaloning in broadband and medium-band imaging scenarios. The Euclid visible instrument is selected as a broadband case study, covering the wavelength range from 550 nm to 900 nm [8]. To show the bandwidth dependent effects of the etaloning, the first channel of the Copernicus Carbon Dioxide Monitoring constellation (CO2M) Cloud Imager is considered, operating at 670 nm with a bandwidth of 20 nm [9]. It should be emphasized that these missions were selected solely because they employ BI-CCD detectors and not due to any specific concerns regarding contamination.

Since contamination layer thicknesses encountered in space environments have not yet been directly characterized for detector surfaces, realistic ranges must be estimated from the available literature. A 1993 study on the effects of spacecraft outgassing products on cryogenic surfaces investigated RTV566 glue contamination layers with thicknesses of up to 1.48 μm [3]. More recent studies, such as [6] and [10], focused on water-ice contamination layers with thicknesses of up to 200 nm. There, contamination accumulation rates of up to 22 nm per month on detector surfaces were reported. Based on these findings, contamination layers with thicknesses of up to 400 nm are considered in this work to assess worst-case contamination-induced etaloning effects. However, to avoid optimizing detector layer thicknesses for highly conservative and potentially unrealistic contamination scenarios, the optimization procedure is limited to contamination layers up to 200 nm thick. Throughout this study, the thicknesses of the native oxide and AR coating layers are varied between 10 nm and 100 nm. The contamination materials considered in this study are water, water ice, carbon, hydrocarbon, siloxane and glues Loctite3526 and RTV615. The refractive indices (n) and extinction coefficients (k) of the BI-CCD and contamination materials were obtained from the Refractiveindex.info database [11], with the exception of the extinction coefficient of RTV615. Details of the optical constant sources used for each material are provided in Table 1.

Table 1: Sources of the wavelength-dependent refractive index and extinction coefficient data used in the simulations [11].

Detector Material	Optical Constants Source	Contamination Material	Optical Constants Source
Silicon	n, k : [12], [13]	Water	n : [16], k : [17]
SiO_2	n, k : [14]	Water Ice	n, k : [18]
HfO_2	n, k : [15]	Siloxane	n, k : [19], [20]
		RTV615	n : [21], k : [22]
		Loctite3526	n : [23], k : unknown
		Carbon	n, k : [24]
		Hydrocarbon	n, k : [25]

Optimization Algorithm

Before optimising the native oxide and AR coating layer thicknesses to minimize contamination-induced etaloning, the detector configuration that maximises transmission into the photosensitive region under contamination-free conditions must first be identified. Therefore, transmission spectra (T) are calculated for all investigated combinations of native oxide and AR-coating thicknesses across the wavelength range $[\lambda_0, \lambda_1]$ of each imaging scenario. The mean transmission, averaged over the respective wavelength range, is then used as the optimisation criterion. The resulting layer thickness combination corresponds to the detector design that provides the highest average transmission without contamination.

To quantify the impact of contamination on the transmission spectra, three metrics are evaluated for an increasing thickness of each contamination material. First, the mean value (T_{mean}) is calculated with Eq. (1) to assess the reduction in the overall transmission level and the associated degradation in the quantum efficiency.

$$T_{mean} = \frac{1}{\lambda_1 - \lambda_0} \sum_{i=\lambda_0}^{\lambda_1} T_i \quad (1)$$

Second, the root-mean-square error ($RMSE$) between the transmission curve with (T_c) and without contamination (T_r) is determined, using Eq. (2). This metric serves as an indicator of the error that would arise if calibration data acquired prior to contamination were applied to measurements affected by contamination-induced etaloning.

$$RMSE = \sqrt{\sum_{i=\lambda_0}^{\lambda_1} \frac{(T_{c,i} - T_{r,i})^2}{\lambda_1 - \lambda_0}} \quad (2)$$

Finally, the number of oscillations (N_{osc}) is evaluated to quantify changes in the fringe pattern. This metric is particularly relevant when the contaminated transmission spectrum oscillates around the uncontaminated reference spectrum, indicating phase shifts and modifications of the etaloning behavior.

For each combination of native oxide, AR-coating, and contamination layer thicknesses (d_c), the three metrics are calculated and subsequently normalised to a range between 0 and 1 across all investigated multilayer stack configurations. Since higher values of T_{mean} correspond to improved detector performance, the normalised T_{mean} values are inverted to ensure that lower scores consistently indicate more favourable designs for all metrics. The three metrics are then combined into a single cost function by calculating their weighted sum (see Eq. (3)), providing a measure of the stability of each detector design to contamination-induced transmission changes. Depending on the application, individual weighting factors (w) can be assigned to emphasise specific performance criteria. In the present study, however, equal weighting is applied to all three metrics.

$$Cost(d_c) = w_{RMSE} * RMSE_{norm}(d_c) + w_{N_{osc}} * N_{osc,norm}(d_c) - w_{T_{mean}} * T_{mean,norm}(d_c) \quad (3)$$

The cost function ($Cost(d_c)$) is subsequently evaluated for increasing contamination layer thicknesses and summed over all investigated thickness values for each contamination material. The detector design with the lowest cumulative cost is identified as the optimum configuration, as it exhibits the smallest sensitivity to contamination-induced changes in transmission and etaloning behavior. The proposed optimisation approach can be performed separately for each contamination material or jointly for the complete set of investigated contaminants.

3. RESULTS

Verification of the Simulation Approach

The paper [2] presents a detailed BI-CCD model represented as a multilayer thin-film stack and calculates the reflection, absorption, and transmission spectra using the same underlying optical formalism implemented in POCAL. To validate the modelling approach adopted in this study, the detector architecture described in [2] was reproduced in POCAL and the resulting spectral characteristics were compared with the published results.

Figure 3 compares the reflection, absorption, and transmission spectra obtained from [2] with those calculated using POCAL. Overall, a good agreement is observed between the two approaches. Differences are mainly visible at wavelengths below 500 nm, where discrepancies occur in the absorption and reflection spectra, and at wavelengths above 900 nm, where deviations are observed in the reflection and transmission spectra. These differences are most likely caused by uncertainties in the optical material properties used in the simulations. Refractive indices and extinction coefficients are not publicly available for all detector materials, requiring approximations in some cases. For example, the in-situ doped polysilicon layer described in [2] was represented by silicon in the present study. Since the silicon detection region has a dominant influence on the optical response of the detector, particular attention was given to the selection of its optical constants. To achieve the closest agreement with the published results, optical data from two sources were combined, using the dataset from [12] below 826.6 nm and the dataset from [13] above 826.6 nm.

This comparison highlights the importance of accurate optical material properties when modelling detector performance. Nevertheless, the overall spectral behavior and trends are reproduced well, particularly within the wavelength ranges relevant to the example missions considered in this paper. The similarity of the resulting reflection, absorption, and transmission spectra demonstrates that the implemented simulation approach provides a valid representation of the detector's optical response. Furthermore, as the objective of this study is to investigate the influence of contamination layers on etaloning and to identify detector layer thickness configurations that mitigate this effect, small inaccuracies in the optical constants do not affect the main conclusions. The underlying physical mechanisms and observed trends remain unchanged.

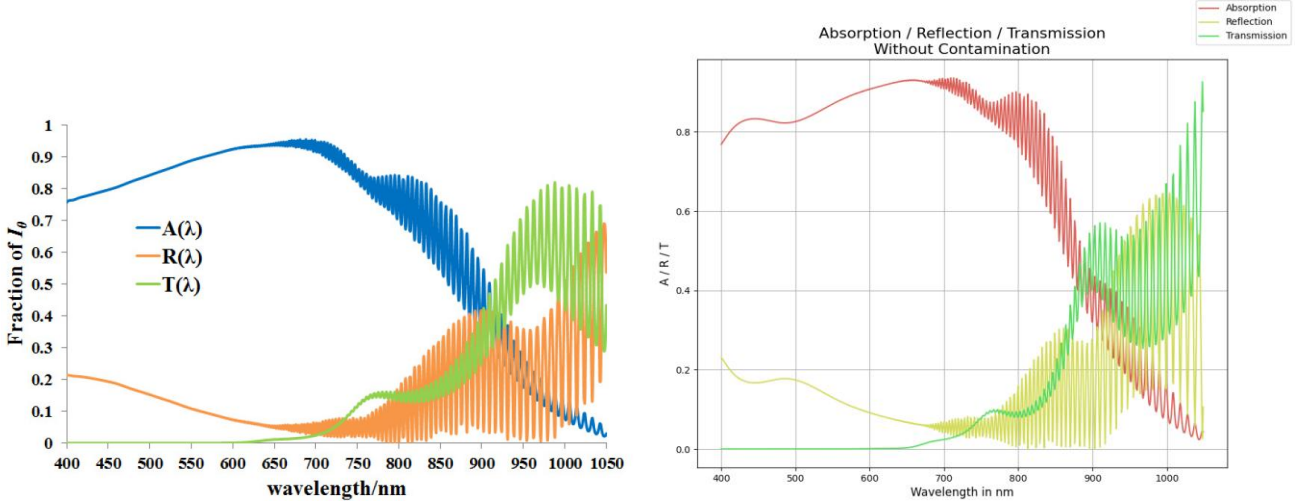


Figure 3: Simulated absorption, reflection and transmission coefficients as a function of wavelength, left: presented in [2], right: result of the algorithm presented in this study

Optimizing the BI-CCD Model without Contamination

For both the broadband and medium-band imaging scenarios, the detector configuration that maximizes the average transmission into the photosensitive region under contamination-free conditions consists of a 25 nm native oxide layer and a 55 nm AR coating. To identify this optimum, the thicknesses of both layers were varied between 10 nm and 100 nm in steps of 5 nm. The resulting mean transmission and standard deviation of the transmission spectrum for the broadband and medium-band cases are summarized below. The transmission spectrum is shown in Figure 4 with the marked wavelength range for the broadband imaging scenario.

- Broadband: $T_{r,mean} \pm \sigma(T_r) = (97.28 \pm 2.40)\%$
- Medium-band: $T_{r,mean} \pm \sigma(T_r) = (99.84 \pm 0.09)\%$

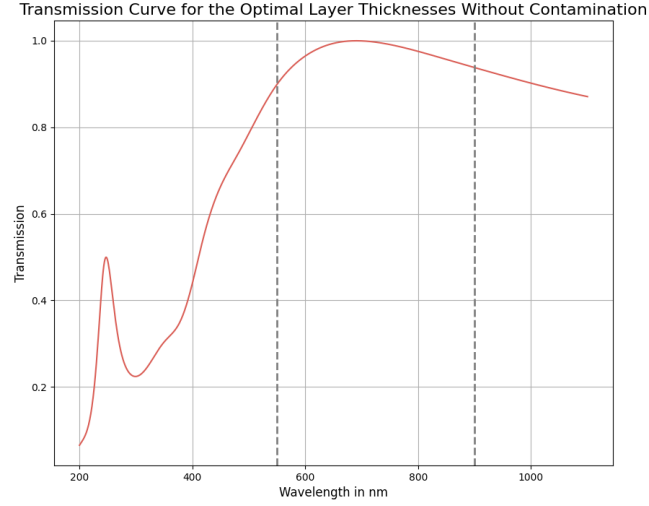


Figure 4: Transmission curve at the photosensitive region with 25 nm SiO₂ thickness and 55 nm HfO₂ thickness without contamination. This layer combination results in the maximum mean value of the transmission over the specified wavelength range for Euclid.

Contamination-Induced Etaloning and Optimizing the BI-CCD Model for a Broadband Mission Scenario

The influence of contamination on the transmission spectra of the detector with 25 nm SiO₂ thickness and 55 nm HfO₂ was investigated for contamination layer thicknesses ranging from 0 to 400 nm. Figure 5 presents the transmission curves over the broadband wavelength range for all considered contaminants and contamination thicknesses up to 200 nm. For all contamination materials, an increase in contamination thickness induces a phase shift of the transmission spectrum towards longer wavelengths. As a result, the positions of the transmission maxima initially move to longer wavelengths relative to the uncontaminated reference spectrum. For larger contamination thicknesses, the periodic nature of thin-film interference causes the transmission maxima to reappear at shorter wavelengths with respect to the reference.

The magnitude of the spectral evolution depends strongly on the optical properties of the contamination material. Around a contamination thickness of approximately 100 nm, the deviation from the reference transmission curve becomes most pronounced for most contaminants. For Loctite 3526 and Hydrocarbon contamination, the spectral shift becomes sufficiently large so that transmission minima occur near wavelengths corresponding to transmission maxima in the reference spectrum. Carbon contamination exhibits a distinctly different behavior due to its comparatively high extinction coefficient, leading to a substantial reduction in transmission across the entire wavelength range and, consequently, a significant degradation of the detector's quantum efficiency.

To quantify the wavelength shift induced by contamination, the transmission maxima were analyzed as a function of contamination thickness. Averaged over contamination layer thicknesses between 5 and 200 nm, the wavelength shifts were found to be 6.89 ± 4.52 nm for Water, 6.68 ± 4.14 nm for Water Ice, 7.24 ± 5.47 nm for Siloxane, 7.29 ± 6.02 nm for RTV615, 7.58 ± 6.93 nm for Loctite 3526, and 8.89 ± 9.43 nm for Hydrocarbon contamination. Carbon exhibited a significantly smaller average wavelength shift of 1.74 ± 10.22 nm. These results indicate that most contaminants produce comparable phase shifts, whereas Carbon primarily affects the overall transmission level through absorption rather than modifying the interference pattern.

To analyze the contamination effects in more detail, the root mean square error ($RMSE$), the mean transmission (T_{mean}), and the number of oscillations (N_{osc}) were calculated for contamination thicknesses up to 400 nm, as shown in Figure 6 for the broadband example mission as orange triangles. For all contaminants except Carbon, the $RMSE$ initially increases

with contamination thickness, reaching a first maximum at contamination thicknesses between 85 nm and 95 nm. These maximum $RMSE$ values are 5.53% for Water at $d_c=85$ nm, 5.03% for Water Ice at $d_c=85$ nm, 6.99% for Siloxane at $d_c=85$ nm, 7.93% for RTV615 at $d_c=90$ nm, 10.25% for Loctite 3526 at $d_c=95$ nm, and 20.98% for Hydrocarbon at $d_c=95$ nm. Carbon contamination does not exhibit a pronounced maximum; instead, its $RMSE$ increases continuously with thickness due to the increasing absorption losses until 96.82% at $d_c=400$ nm. Following the first maximum, the $RMSE$ remains relatively stable for most contaminants, with average values of 6.36% for Water, 4.06% for Water Ice, 5.81% for Siloxane, 6.58% for RTV615, and 8.30% for Loctite 3526. Hydrocarbon contamination shows a different behavior, with the $RMSE$ decreasing again before 200 nm and subsequently increasing to 21.52% at 400 nm.

The mean transmission of the uncontaminated detector is 97.28%. For all contaminants except Carbon, T_{mean} initially decreases with contamination thickness, reaching a first minimum before exhibiting an oscillatory behavior caused by the thin-film interference. The minimum mean transmission values are 94.03% for Water at $d_c=125$ nm, 94.65% for Water Ice at $d_c=125$ nm, 92.21% for Siloxane at $d_c=120$ nm, 91.05% for RTV615 at $d_c=120$ nm, 88.52% for Loctite 3526 at $d_c=115$ nm, and 77.14% for Hydrocarbon at $d_c=100$ nm. Carbon contamination again shows a fundamentally different trend, with the mean transmission decreasing continuously and reaching 0.49% at $d_c=400$ nm.

The number of oscillations, N_{osc} , generally increases with increasing contamination thickness for all contaminants. Small decreases can be observed at specific thicknesses, corresponding to phase shifts that move transmission maxima or minima into or out of the analyzed wavelength range. Overall, the increase in N_{osc} reflects the growing optical path length introduced by the contamination layer and the resulting increase in contamination-induced etaloning across the investigated spectral range.

These results demonstrate that contamination can significantly modify both the average transmission and the interference structure of backside-illuminated detectors. While highly absorbing contaminants such as Carbon primarily reduce transmission, transparent contaminants induce wavelength shifts and changes in the etaloning pattern that may substantially alter the detector response, particularly for contamination thicknesses around 100 nm where the spectral deviations are largest.

To improve the contamination tolerance of the BI-CCD design, the thicknesses of the native oxide (SiO_2) and AR coating (HfO_2) layers were optimized for each contaminant individually. The resulting layer configurations and their corresponding performance metrics are presented in the following sections. The objective of the optimization was to decrease contamination-induced transmission degradation while maintaining a high overall transmission performance. To reduce computational effort, the contamination thickness step size was increased to 25 nm, and the optimization procedure was limited to contamination thicknesses up to 200 nm. The resulting optimized SiO_2 and HfO_2 layer thicknesses for each contaminant are summarized in Table 2. During the optimization, the SiO_2 thickness was varied between 10 nm and 45 nm and the HfO_2 thickness between 35 nm and 75 nm, both with a step size of 5 nm. In addition to the optimized layer thicknesses, Table 2 lists the mean transmission and standard deviation of the uncontaminated transmission spectrum for each optimized BI-CCD configuration. The reference detector design, consisting of a 25 nm SiO_2 layer and a 55 nm HfO_2 layer, was previously identified as providing the highest average transmission in the absence of contamination, reaching $T_{mean} = 97.28\%$. Compared with this reference configuration, the optimized detector designs generally exhibit a lower uncontaminated transmission and a larger standard deviation of the transmission spectrum. This observation highlights the trade-off introduced by the optimization process. Although the optimized BI-CCD configurations exhibit a lower initial transmission performance in the absence of contamination, they are designed to be less susceptible to contamination-induced degradation. To assess the effectiveness of the optimization and illustrate this trade-off, the $RMSE$, T_{mean} , and N_{osc} were recalculated for contamination thicknesses up to 400 nm using the optimized BI-CCD layer configurations for each contaminant. The corresponding results are presented in Figure 6 (blue markers).

Table 2: Detector layer thicknesses optimized for different contamination scenarios and the mean and standard deviation of these designs without contamination between 550 and 900 nm wavelength range for the broadband example mission.

Optimization Item for Broadband Example Mission	Thickness of SiO ₂ Layer in nm	Thickness of HfO ₂ Layer in nm	Mean Transmission without Contamination in %	STD Transmission without Contamination in %
Without Contamination	25	55	97.28	2.40
Water	10	65	96.70	2.66
Water Ice	20	70	95.66	5.32
Siloxane	10	65	96.70	2.66
Loctite 3526	10	55	93.64	4.38
RTV615	10	75	96.90	2.95
Carbon	45	75	77.66	14.24
Hydrocarbon	10	45	88.32	4.64

The *RMSE* values of the optimized BI-CCD models initially increases with the contamination thickness for all contaminants except Carbon, reaching a first maximum between approximately 65 and 115 nm. Compared with the non-optimized detector configuration, these first maxima of the *RMSE* are significantly reduced. Peak *RMSE* values of 4.87%, 3.96%, 5.78%, 5.60%, 8.80%, and 13.96% are obtained for Water, Water Ice, Siloxane, RTV615, Loctite3526, and Hydrocarbon contamination, respectively. These maxima occur at contamination thicknesses of 85 nm, 65 nm, 85 nm, 75 nm, 90 nm, and 115 nm. For Carbon contamination, the overall *RMSE* trend remains similar to that observed for the non-optimized detector design; however, the absolute *RMSE* values are substantially lower. At a contamination thickness of 400 nm, the *RMSE* reaches 78.38%, compared with 96.82% for the non-optimized configuration. For Water, Siloxane, and RTV615 contamination, the *RMSE* remains relatively constant after the first maximum, with average values of approximately 3.50%, 4.51%, and 5.00%, respectively. These levels are consistently lower than those obtained with the non-optimized detector design. Loctite3526 and Hydrocarbon exhibit stronger *RMSE* fluctuations over the contamination thickness range, but their *RMSE* values remain below those of the non-optimized configuration. For Water Ice, the optimized design generally yields lower *RMSE* values than the non-optimized detector, with an average difference of approximately 0.7%. An exception is observed for contamination thicknesses between 125 and 200 nm, where the optimized configuration produces slightly larger *RMSE* values.

The behavior of T_{mean} differs between contaminants. For Water, Siloxane, Loctite3526, and Hydrocarbon, the mean transmission initially increases for thin contamination layers before reaching a minimum at larger thicknesses. For Water, T_{mean} increases to 97.62% at a contamination thickness of 50 nm before decreasing to a minimum of 93.96% at 240 nm. Similar behavior is observed for Siloxane, where T_{mean} reaches a maximum of 97.47% at 35 nm and a minimum of 93.18% at 215 nm. For Loctite3526, a maximum transmission of 97.79% is obtained at 45 nm, followed by a minimum of 87.92% at 165 nm. Hydrocarbon contamination exhibits the strongest degradation, with T_{mean} increasing to 96.55% at 40 nm before decreasing to 76.43% at 145 nm. Although the maximum transmission degradation for Water, Loctite3526, and Hydrocarbon remains significant, the contamination thickness at which the minimum transmission occurs is shifted towards larger values compared with the non-optimized detector design, indicating an increased tolerance to contamination growth. RTV615 exhibits a different behavior. For thin contamination layers, T_{mean} decreases and remains below the corresponding values of the non-optimized detector. However, the minimum transmission of 93.08% is reached at a contamination thickness of 95 nm, after which the optimized design provides consistently higher transmission values than the non-optimized configuration. For Water Ice contamination, the average T_{mean} over the entire contamination thickness range is lower for the optimized detector design than for the non-optimized configuration. However, the corresponding N_{osc} values are reduced for contamination thicknesses between approximately 75 and 125 nm. This result indicates that the applied optimization strategy successfully improves some transmission characteristics for most contaminants, but not necessarily all performance metrics simultaneously. A more detailed assessment of the transmission metrics and their relative weighting may therefore be required to tailor the optimization to specific mission requirements. The mean

transmission for Carbon contamination changes only marginally with increasing contamination thickness and follows a similar increasing trend to that observed for the non-optimized detector design.

Overall, the optimization procedure reduces the susceptibility of the BI-CCD design to contamination-induced etaloning for most contaminants, primarily by lowering *RMSE* levels and delaying the significant transmission degradation to larger contamination thicknesses.

In addition to the transmission metrics, the transmission spectra of the optimized BI-CCD configurations under contamination are shown in Figure 7 for contamination thicknesses up to 200 nm. Similar to the non-optimized detector design, the spectra exhibit a phase shift towards longer wavelengths as the contamination thickness increases, accompanied by a degradation of the transmission. However, the magnitude of these effects is generally reduced, consistent with the improvements observed in the *RMSE* and T_{mean} metrics. Furthermore, the wavelength shift induced by a 5 nm contamination layer was evaluated for the optimized BI-CCD configurations for the broadband example mission. The average wavelength shifts over contamination thicknesses between 5 nm and 200 nm were calculated. The optimization of the BI-CCD layer thicknesses does not generally improve the wavelength shift behavior, despite the observed reductions in *RMSE* and improvements in T_{mean} . For several contaminants, the average wavelength shift even increases after optimization. Water, Siloxane, Loctite3526, Carbon, and Hydrocarbon exhibit larger average wavelength shifts after optimization, increasing from $6.89 \pm 4.52\text{nm}$ to $7.82 \pm 4.80\text{nm}$, $7.24 \pm 5.47\text{nm}$ to $7.95 \pm 5.74\text{nm}$, $7.58 \pm 6.93\text{nm}$ to $9.39 \pm 8.81\text{nm}$, $1.74 \pm 10.22\text{nm}$ to $6.55 \pm 6.37\text{nm}$, and $8.89 \pm 9.43\text{nm}$ to $11.21 \pm 12.05\text{nm}$, respectively. Only Water Ice and RTV615 show a slight reduction in the average wavelength shift after optimization. For Water Ice, the shift decreases from $6.68 \pm 4.14\text{nm}$ to $4.47 \pm 3.89\text{nm}$, while RTV615 exhibits a marginal reduction from $7.29 \pm 6.02\text{nm}$ to $7.03 \pm 5.15\text{nm}$. These results indicate that minimizing contamination-induced etaloning and maximizing transmission performance does not necessarily reduce spectral wavelength shifts. The optimization procedure was designed to minimize *RMSE*, maximise T_{mean} , and reduce oscillatory behavior, but wavelength stability was not included as an optimization criterion. This highlights the need for mission-specific optimization strategies when spectral accuracy is a critical performance requirement. In such cases, wavelength shift should be incorporated as an additional term in the optimization cost function.

In practice, it can be expected that more than one contamination material is present on a detector during a mission. Therefore, the optimization procedure was also applied simultaneously to all considered contaminants in order to identify a BI-CCD configuration that provides reduced sensitivity against contamination-induced transmission degradation for the complete contamination set. The resulting optimal detector design consists of a 10 nm SiO_2 layer and a 40 nm HfO_2 layer. The corresponding transmission metrics are shown as blue markers in Figure 8. Compared with the reference BI-CCD configuration (orange triangles), the optimized detector generally exhibits poorer transmission metric values for most contaminants. An exception is observed for Hydrocarbon and Carbon contamination, for which the optimized design provides a noticeable improvement. As these two contaminants have material properties that differ significantly from those of the remaining contaminants, they strongly influence the optimisation result when all contaminants are weighted equally within the cost function. To further investigate this effect, the optimization was repeated with Carbon excluded from the cost function. In this case, the optimal detector design was found to consist of a 10 nm SiO_2 layer and a 65 nm HfO_2 layer. The resulting transmission metrics are shown as green markers in Figure 8. With the exception of Carbon contamination, this detector configuration exhibits a substantially lower susceptibility to contamination-induced etaloning across all considered contaminants. These results demonstrate that the optimum detector design strongly depends on the assumed contamination environment and underline the importance of realistic contamination assessments during detector design and optimization. In particular, contaminants with strongly differing optical properties can dominate the optimization process and bias the resulting layer configuration if all contaminants are weighted equally.

Contamination-Induced Etaloning and Optimizing the BI-CCD Model for a Medium-Band Mission Scenario

To assess the influence of contamination on the transmission characteristics of the BI-CCD model before applying any optimization for the smaller wavelength band, the root mean square error (*RMSE*), mean transmission (T_{mean}), and number of oscillations (N_{osc}) were calculated analogously to the broadband mission scenario, but within the wavelength range from 660 nm to 680 nm. The results are presented in Figure 9 as orange triangles.

For all contaminants except Carbon, the *RMSE* initially increases with contamination thickness, reaching a first maximum between 90 and 115 nm. Subsequently, the *RMSE* decreases to a minimum between approximately 185 and 255 nm before

increasing again for larger contamination thicknesses. The first *RMSE* maxima are 7.78%, 6.91%, 10.23%, 11.66%, 14.94%, and 27.30% for Water, Water Ice, Siloxane, RTV615, Loctite3526, and Hydrocarbon contamination, respectively. These peaks occur at contamination thicknesses between 90 and 115 nm. The corresponding minima range from 0.05% to 4.36% and are reached at contamination thicknesses between 185 and 255 nm. Hydrocarbon exhibits the strongest contamination impact, with a first *RMSE* maximum of 27.30% at $d_c = 90\text{nm}$ and a minimum of 4.36% at $d_c = 185\text{nm}$. Carbon contamination shows a distinctly different behavior. Instead of exhibiting periodic maxima and minima, the *RMSE* increases continuously with contamination thickness and reaches 99.50% at $d_c = 400\text{nm}$.

The behavior of the mean transmission is inversely correlated with that of the *RMSE*. Owing to the narrow wavelength range considered, the transmission spectra exhibit little to no oscillatory behavior, resulting in a strong correlation between T_{mean} and *RMSE*. Consequently, N_{osc} remains close to zero for all contaminants and never exceeds one oscillation over the analyzed wavelength interval. Starting from an uncontaminated mean transmission of 99.84%, Water contamination causes T_{mean} to decrease to a first minimum of 92.05% at $d_c = 115\text{nm}$ before increasing again to 99.96% at $d_c = 240\text{nm}$. Similar behavior is observed for Water Ice, with a minimum of 92.93% at 115 nm and a maximum of 99.97% at 245 nm. Siloxane, RTV615, and Loctite3526 reach minimum transmission values of 89.61%, 88.18%, and 84.90%, respectively, before recovering to approximately 99.95–99.96% at contamination thicknesses around 225–240 nm. Hydrocarbon exhibits the largest reduction in transmission, decreasing to 72.53% at $d_c = 90\text{nm}$ before increasing to 99.95% at $d_c = 215\text{nm}$. In contrast, Carbon contamination results in a continuous degradation of the mean transmission with increasing contamination thickness. T_{mean} steadily decreases from 99.84% to only 0.34% at $d_c = 400\text{nm}$, reflecting the strong absorption characteristics of Carbon and the absence of the interference-driven behavior observed for the other contaminants.

Overall, the medium-band analysis reveals that contamination-induced interference effects produce alternating regions of transmission degradation and recovery for most contaminants. In contrast to the broadband case, the small wavelength range results in negligible oscillatory behavior, making *RMSE* and mean transmission the dominant performance indicators. Carbon remains the most critical contaminant, causing a nearly monotonic decrease of detector performance over the investigated contamination thickness range.

The optimization procedure was subsequently applied to the medium-band mission scenario. The resulting optimized SiO_2 and HfO_2 layer thicknesses for each contaminant are summarized in Table 3, together with the mean transmission and standard deviation of the uncontaminated transmission spectra. Similar to the broadband case, the optimization aims to reduce the sensitivity of the BI-CCD design to contamination-induced transmission degradation, even if this may require a slight reduction in transmission performance under contamination-free conditions. To evaluate the effectiveness of the optimized detector configurations, the *RMSE*, mean transmission (T_{mean}), and number of oscillations (N_{osc}) were recalculated for contamination thicknesses up to 400 nm. The resulting metrics are presented in Figure 9 (blue markers) and compared with the non-optimized detector design.

Table 3: Detector layer thicknesses optimized for different contamination scenarios and the mean and standard deviation of these designs without contamination between 660 and 680 nm wavelength range for the medium-band example mission.

Optimization Item for Medium-Band Example Mission	Thickness of SiO_2 Layer in nm	Thickness of HfO_2 Layer in nm	Mean Transmission without Contamination in %	STD Transmission without Contamination in %
Without Contamination	25	55	99.84	0.09
Loctite 3526	10	55	96.34	0.28
Water	10	65	99.51	0.10
Water Ice	10	65	99.51	0.10
Siloxane	10	65	99.51	0.10
RTV615	10	75	98.79	0.20
Carbon	45	75	70.82	0.99
Hydrocarbon	10	45	90.36	0.31

For Water, Water Ice, and Siloxane contamination, the optimized detector exhibits a behavior similar to that observed for the non-optimized configuration. However, the maximum $RMSE$ values and minimum T_{mean} values occur at larger contamination thicknesses and are reduced in magnitude. For Water contamination, the $RMSE$ reaches a maximum of 5.09% at $d_c = 145\text{nm}$, while T_{mean} decreases to a minimum of 94.43% at the same contamination thickness. Water Ice contamination results in a maximum $RMSE$ of 4.37% and a minimum T_{mean} of 95.15%, both occurring at $d_c = 150\text{nm}$. For Siloxane, the maximum $RMSE$ is 7.17% and the minimum T_{mean} is 92.34%, reached at $d_c = 135\text{nm}$. In addition, the optimized detector design provides a high degree of stability for contamination thicknesses below 50 nm. Averaged over this thickness range, $RMSE$ values remain below 0.5%, while mean transmission remains above 99.3%. Specifically, average $RMSE$ values of 0.27%, 0.25%, and 0.40% are obtained for Water, Water Ice, and Siloxane contamination, respectively, corresponding to average mean transmission values of 99.60%, 99.66%, and 99.39%. For RTV615 contamination, T_{mean} also decreases with increasing contamination thickness but to a lesser extent than in the non-optimized case. The minimum transmission of 90.39% is reached at $d_c = 95\text{nm}$. The $RMSE$ initially increases and reaches 8.41% at the same contamination thickness. Subsequently, between contamination thicknesses of approximately 185 nm and 235 nm, the $RMSE$ remains below 1.08% before increasing again for thicker contamination layers. This behavior indicates a substantial reduction of contamination-induced transmission degradation over a wide thickness range. Loctite3526 and Hydrocarbon contamination exhibit a different trend. Similar to the non-optimized detector design, T_{mean} initially increases before decreasing to a minimum at larger contamination thicknesses. Minimum transmission values of 85.73% and 72.80% are reached at contamination thicknesses of 145 nm and 130 nm for Loctite3526 and Hydrocarbon, respectively. The corresponding $RMSE$ curves show two distinct local maxima. For Loctite3526 contamination, a first maximum of 3.65% occurs at $d_c = 35\text{nm}$, followed by a second and larger maximum of 10.61% at $d_c = 145\text{nm}$. Hydrocarbon exhibits a similar behavior, with a first maximum of 8.42% at $d_c = 35\text{nm}$ and a second maximum of 17.56% at $d_c = 130\text{nm}$. Despite the presence of these peaks, the $RMSE$ values remain consistently below those obtained for the non-optimized detector configuration. For Carbon contamination, the optimization reduces the overall $RMSE$ across the investigated contamination thickness range. At $d_c = 400\text{nm}$, the $RMSE$ reaches 70.46%, compared with 99.50% for the non-optimized detector design. In contrast, the mean transmission is only marginally influenced by the BI-CCD optimization, indicating that the dominant degradation mechanism for Carbon contamination is largely independent of the detector layer configuration.

Overall, the optimization procedure increases the contamination tolerance of the BI-CCD design for most contaminants by reducing peak $RMSE$ values and shifting the significant transmission degradation towards larger contamination thicknesses. The improvements are particularly pronounced for Water, Water Ice, Siloxane, and RTV615 contamination, while Carbon remains the most challenging contaminant despite a noticeable reduction in $RMSE$.

4. CONCLUSION

This paper presented an optimization approach for identifying the native oxide and AR coating thicknesses of a representative BI-CCD that reduce sensitivity against contamination-induced etaloning. The method determines detector layer configurations that minimize changes in the transmission spectrum caused by contamination layers while maintaining high detector performance. The simulation approach has been validated by comparing the absorption, reflection and transmission coefficients over the wavelength with another publication. Two representative mission scenarios were investigated: a broadband imaging application (550–900 nm) and a medium-band imaging application (660–680 nm). For each scenario, transmission spectra were simulated for BI-CCD configurations exposed to contamination layers of Water, Water Ice, Siloxane, glues RTV615 and Loctite 3526, Hydrocarbon, and Carbon. The transmission behavior was evaluated for contamination thicknesses up to 400 nm using the *RMSE*, mean transmission (T_{mean}), and the number of oscillations (N_{osc}). The optimized detector architectures were compared with the reference BI-CCD design that maximises the transmission without considering any contamination.

It is demonstrated that contamination can significantly affect both the average transmission and the spectral interference characteristics of backside-illuminated detectors. While highly absorbing contaminants mainly reduce transmission, transparent contaminants can induce wavelength shifts and modify the etaloning pattern, leading to substantial changes in detector response. The strongest effects were observed for contamination thicknesses of approximately 100 nm for the broadband application.

For the broadband mission scenario, the optimization reduced the maximum observable *RMSE* for all contaminants except Carbon, with reductions ranging from 0.66% for Water to 7.02% for Hydrocarbon. When optimized individually for each contaminant, the mean *RMSE* for contamination thicknesses larger than 90 nm was reduced to 2.86%, 1.30%, and 1.58% for Water, Siloxane, and RTV615, respectively. For Carbon, the *RMSE* was reduced by 18.44%. These improvements decrease the discrepancy between on-ground calibrated transmission spectra and contamination-affected on-ground or in-flight spectra, thereby reducing contamination-related measurement errors. Furthermore, the optimization improved transmission stability by reducing the maximum degradation of T_{mean} for Siloxane and RTV615 by 0.97% and 2.03%, respectively, while shifting the minimum T_{mean} towards larger contamination thicknesses for Water, Loctite 3526, and Hydrocarbon. For the medium-band mission scenario, the optimized BI-CCD configuration significantly reduced the maximum *RMSE* for all contaminants, with improvements ranging from 2.54% for Water Ice to 9.74% for Hydrocarbon up until 29.04% for Carbon. In addition, the minimum T_{mean} increased by between 0.27% for Hydrocarbon and 2.73% for Siloxane. An additional optimization strategy was presented to identify a single detector configuration that provides improved performance across all considered contaminants. The results show that the optimal solution depends strongly on the optical properties of the contaminating materials. Consequently, a detailed contamination assessment during mission design is essential to identify the most likely contaminant species and their expected thickness evolution throughout the mission lifetime.

Although the optimized detector designs generally exhibit lower uncontaminated transmission than the reference configuration, they show a more stable spectral behavior in the presence of deposited contaminants. This highlights the trade-off between maximizing nominal optical throughput and reduced sensitivity to contamination-induced spectral deviations. As discussed, the operational risk associated with contamination can be mitigated by dedicated detector heaters. In addition, the simulation results demonstrate that accounting for contamination during the detector design phase can significantly reduce etaloning effects, improve transmission stability, and decrease the resulting measurement errors.

The study also highlights the importance of accurate detector and contamination material parameters. Properties such as refractive index, extinction coefficient, and layer thickness have a significant influence on the predicted transmission spectra and therefore on the optimization outcome. As a result, reliable optical material data and detailed knowledge of the detector architecture are key prerequisites for accurately modelling contamination effects. Furthermore, if the detector design is known, the thin-film modelling approach and optimization framework can be used to interpret contamination-related effects observed in flight. By reproducing measured spectral signatures through simulated contamination scenarios, the method enables the reverse engineering of potential contamination layers and degradation mechanisms. The capability can support the identification of likely contamination sources and aid the development of mitigation strategies for future missions.

5. APPENDIX

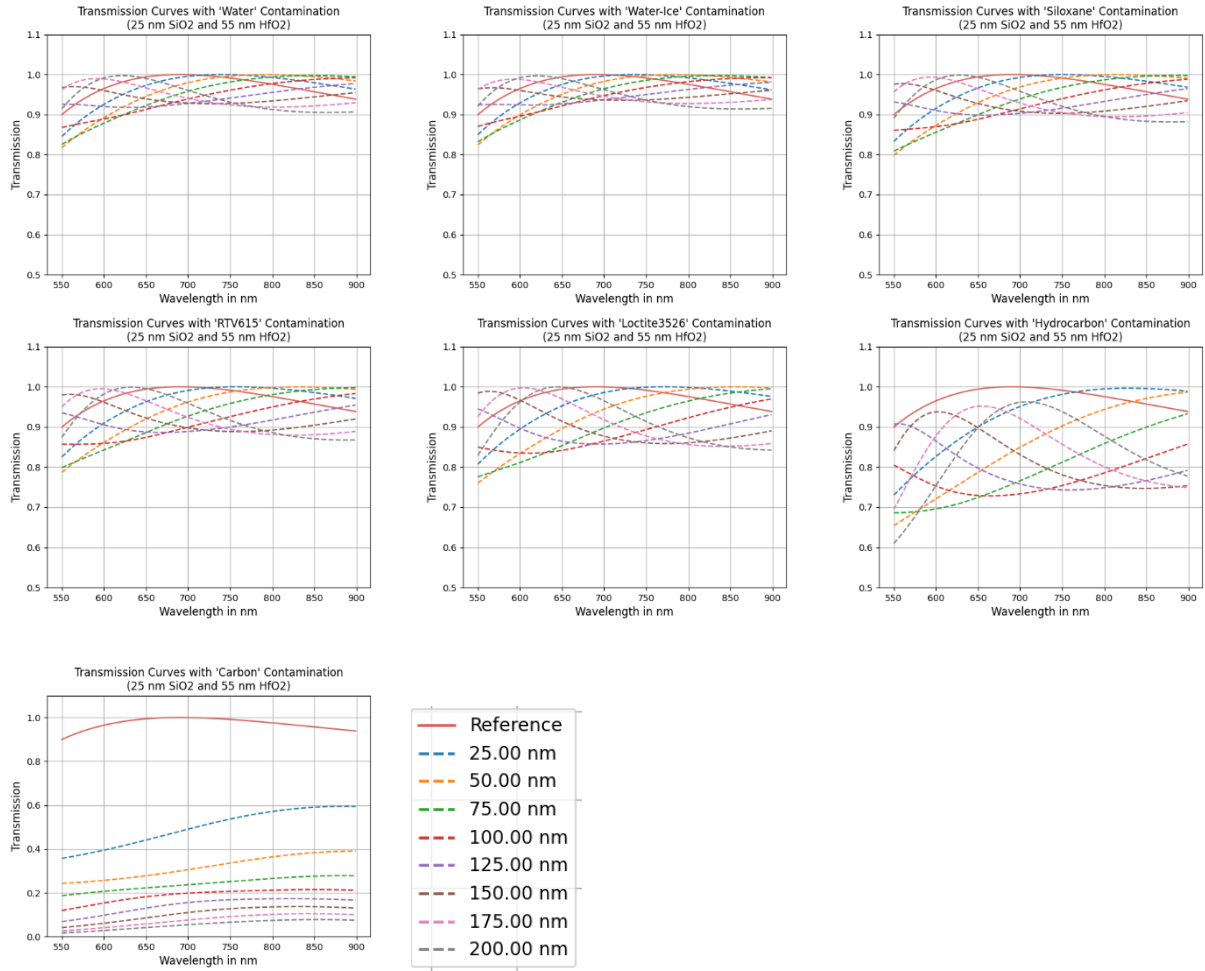
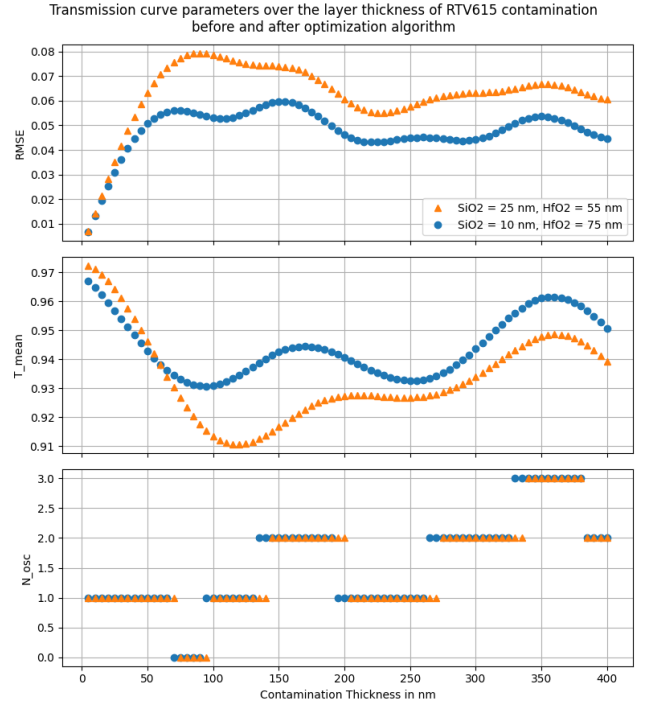
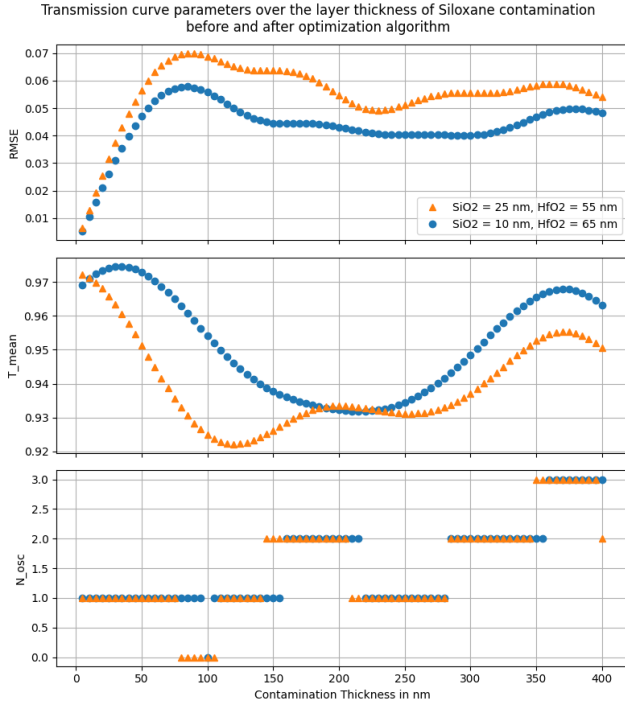
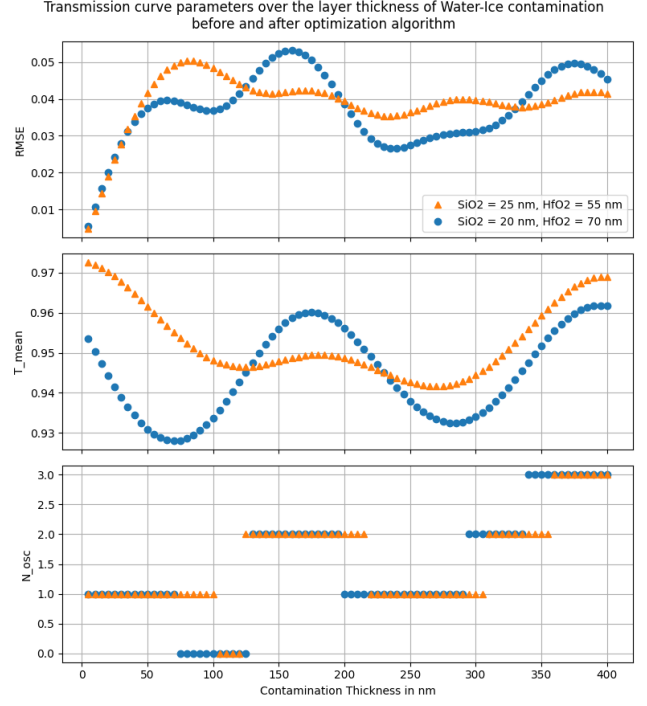
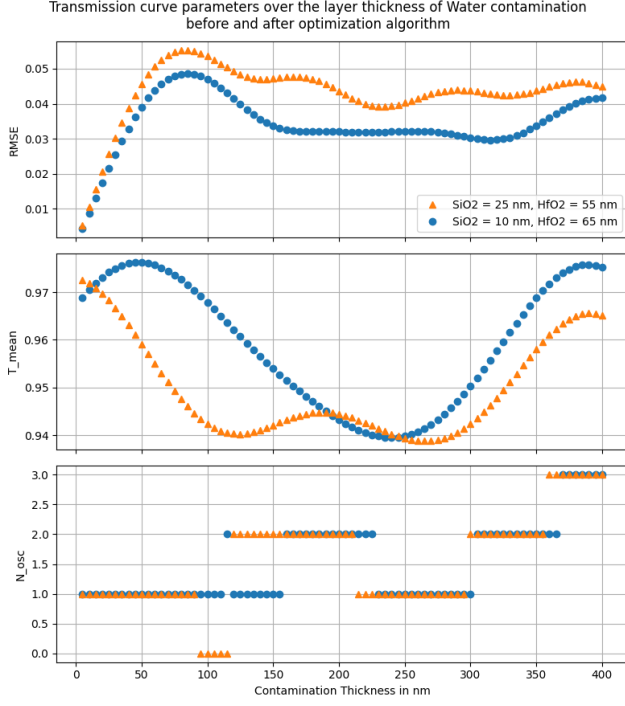


Figure 5: Transmission curve at the photosensitive region with 25 nm SiO₂ thickness and 55 nm HfO₂ thickness with increasing layer thicknesses of different contamination materials.



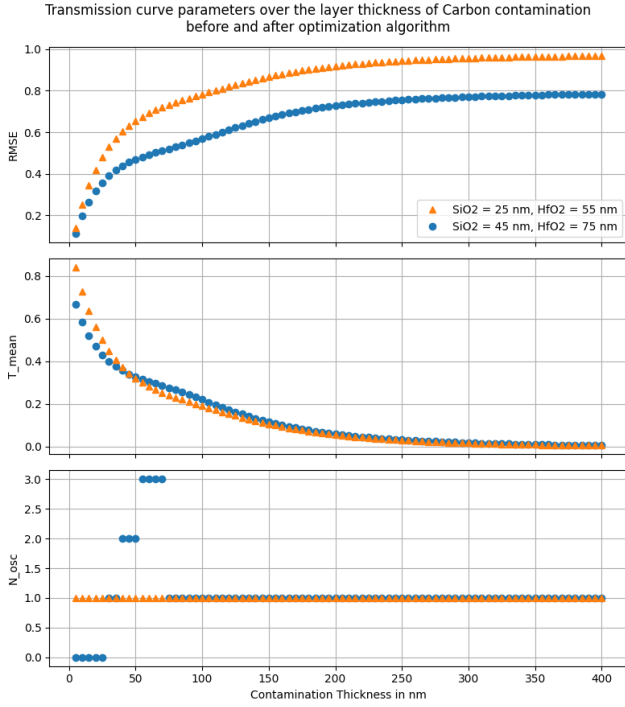
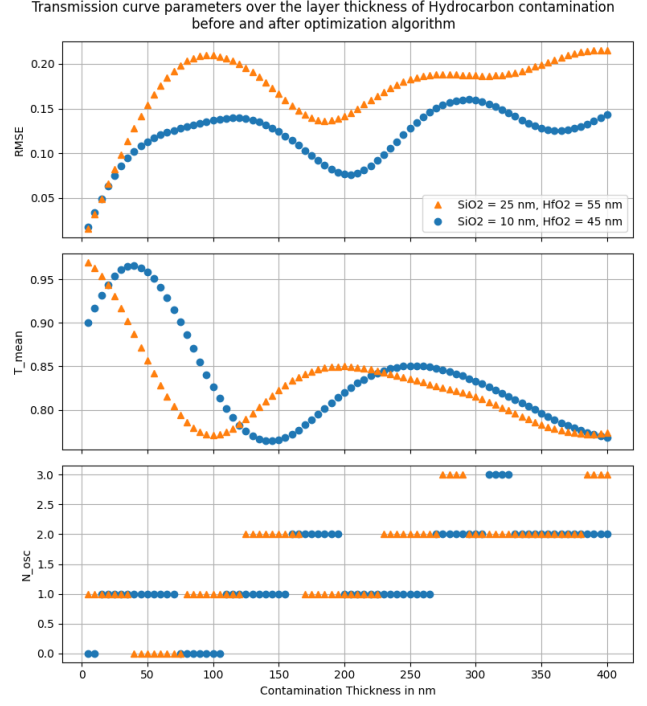
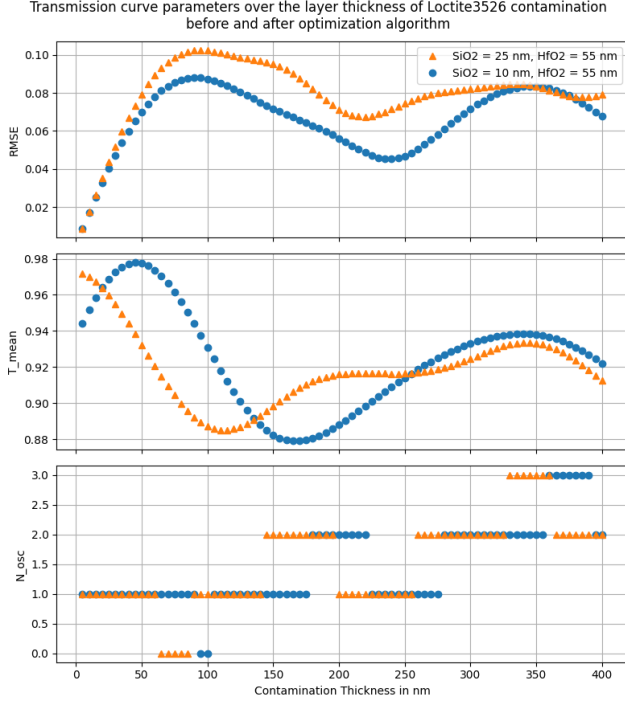


Figure 6: Parameters of the transmission curve at the photosensitive region over the layer thicknesses of different contamination materials for the layer thicknesses of the SiO₂ and HfO₂ layers before and after the optimization algorithm, for the broadband example mission.

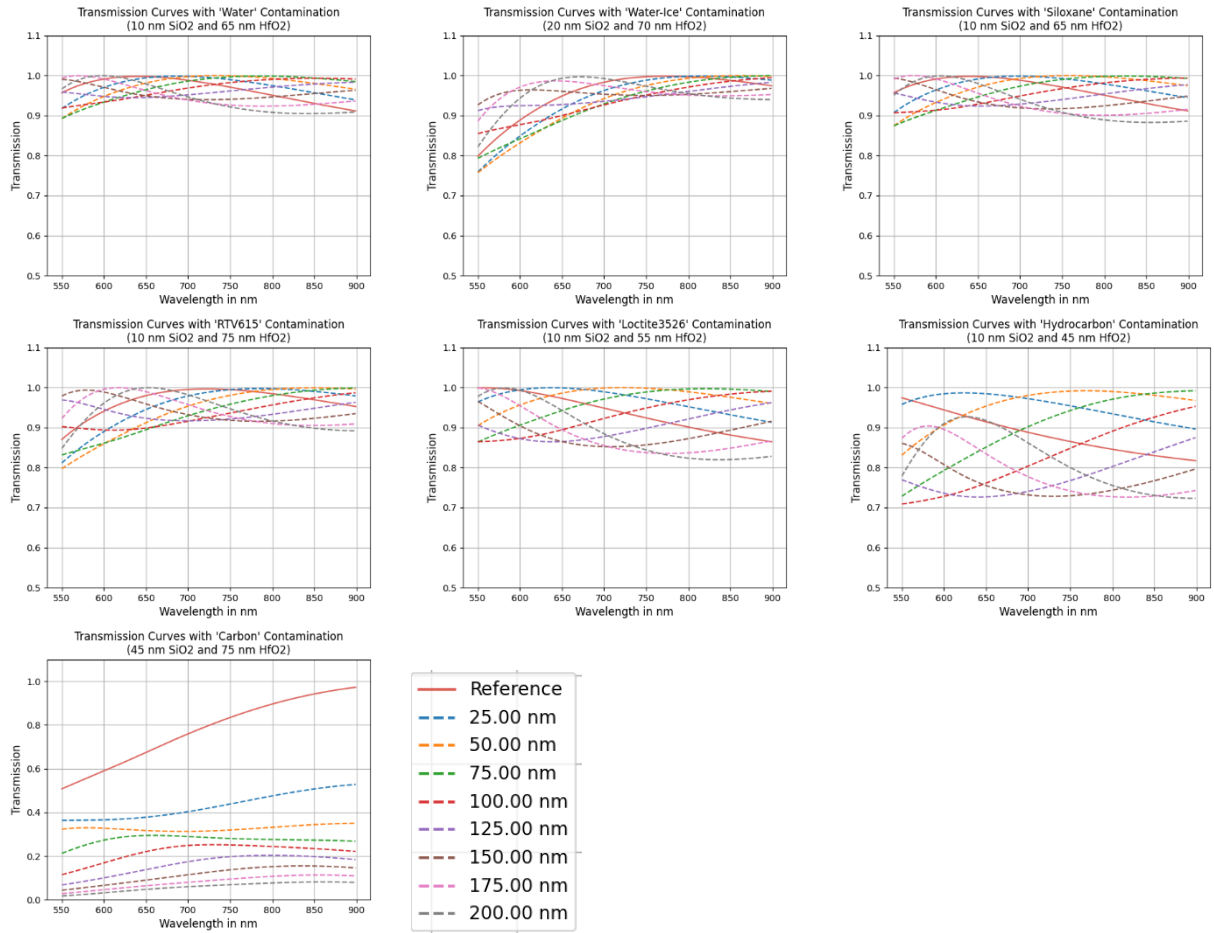
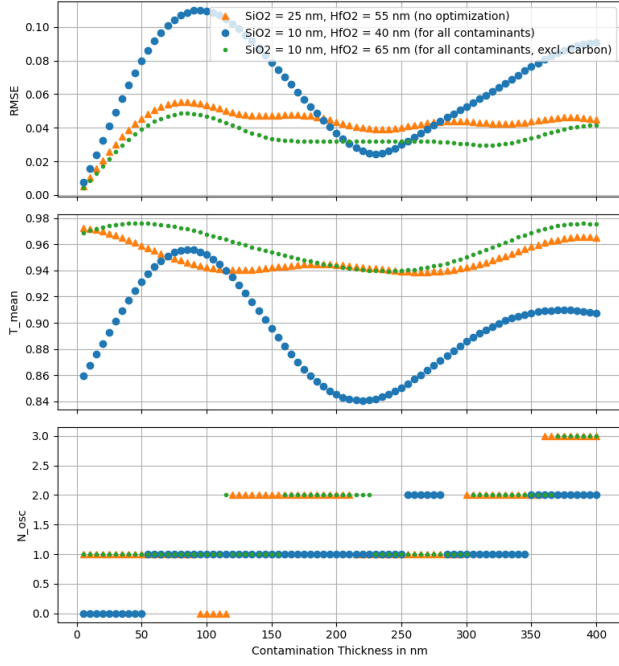
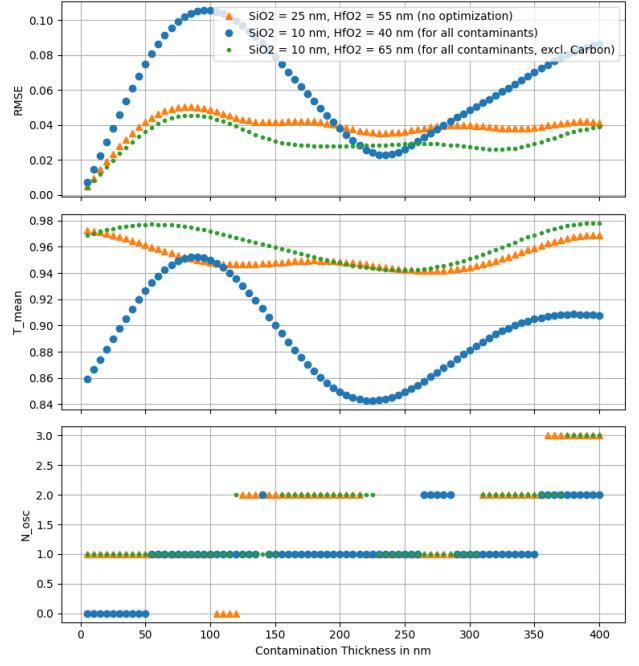


Figure 7: Transmission curve at the photosensitive region with increasing layer thicknesses of different contamination materials. The layer thicknesses of the SiO₂ and HfO₂ layers are optimized for each contamination material, for the broadband example mission.

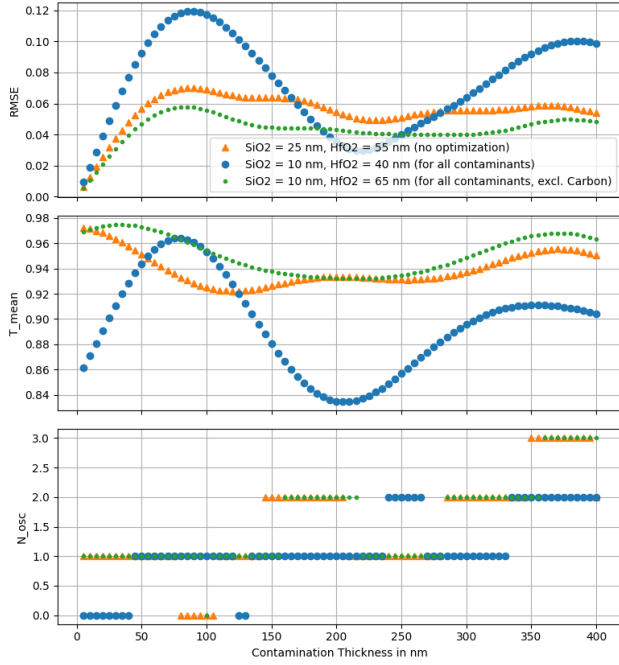
Transmission curve parameters over the layer thickness of Water contamination before and after optimization algorithm



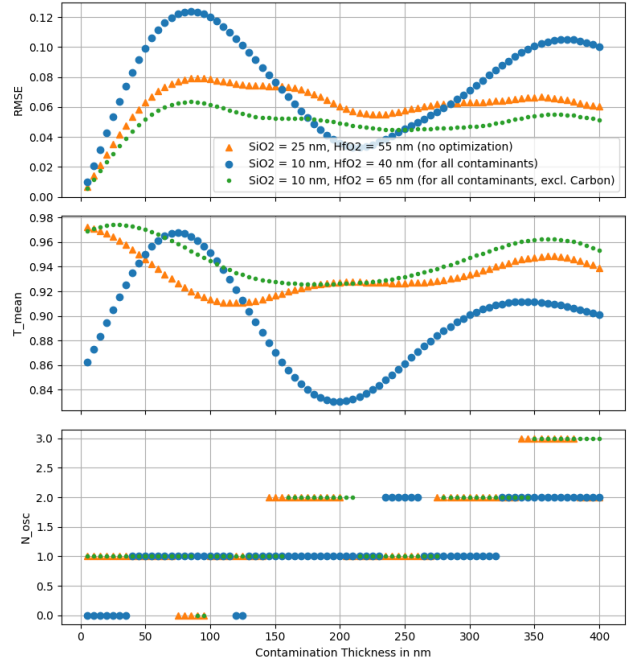
Transmission curve parameters over the layer thickness of Water-Ice contamination before and after optimization algorithm



Transmission curve parameters over the layer thickness of Siloxane contamination before and after optimization algorithm



Transmission curve parameters over the layer thickness of RTV615 contamination before and after optimization algorithm



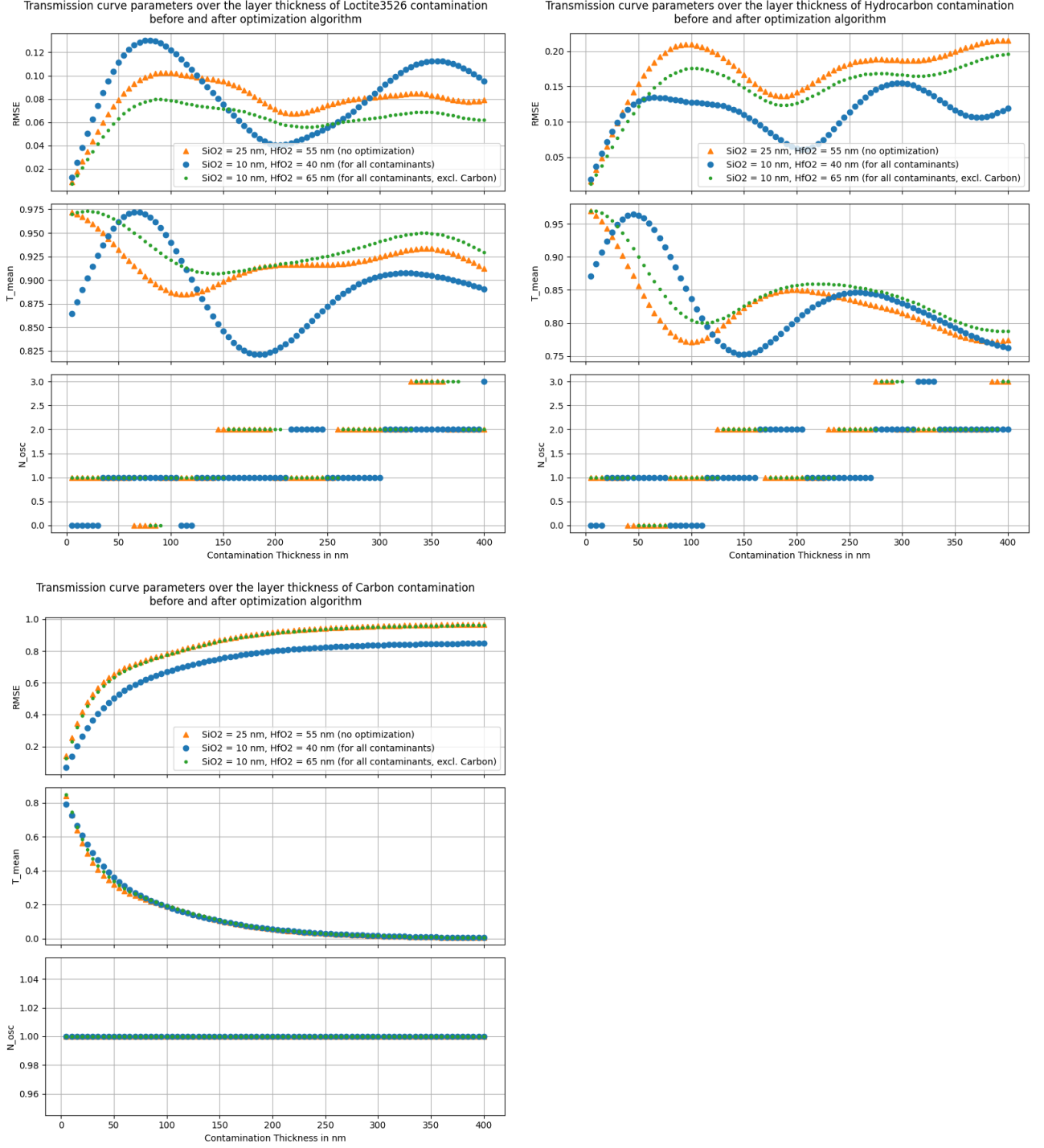
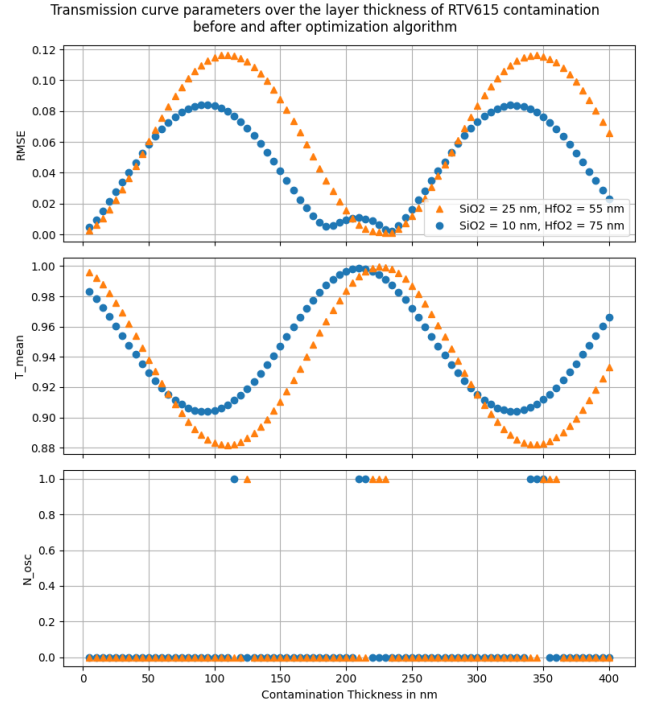
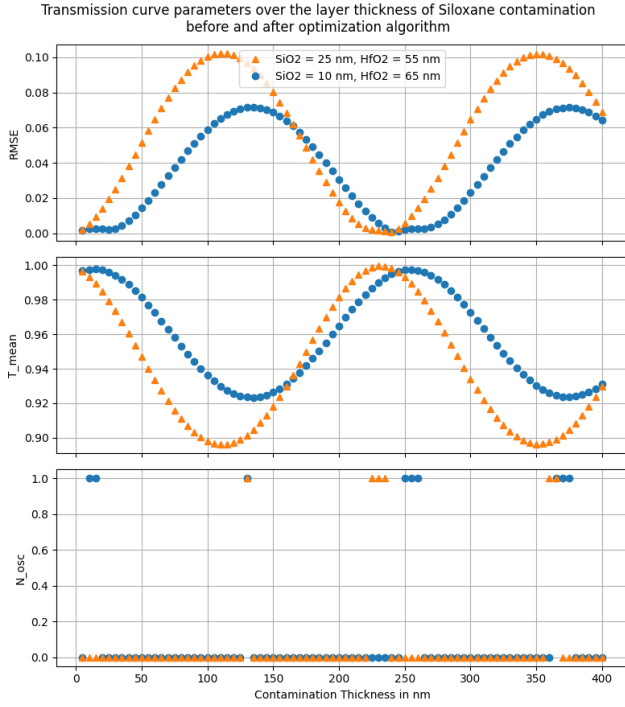
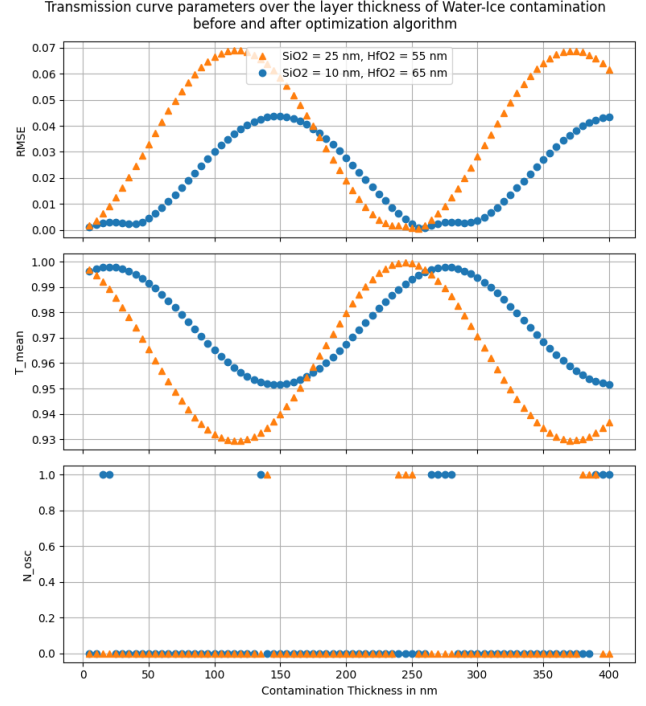
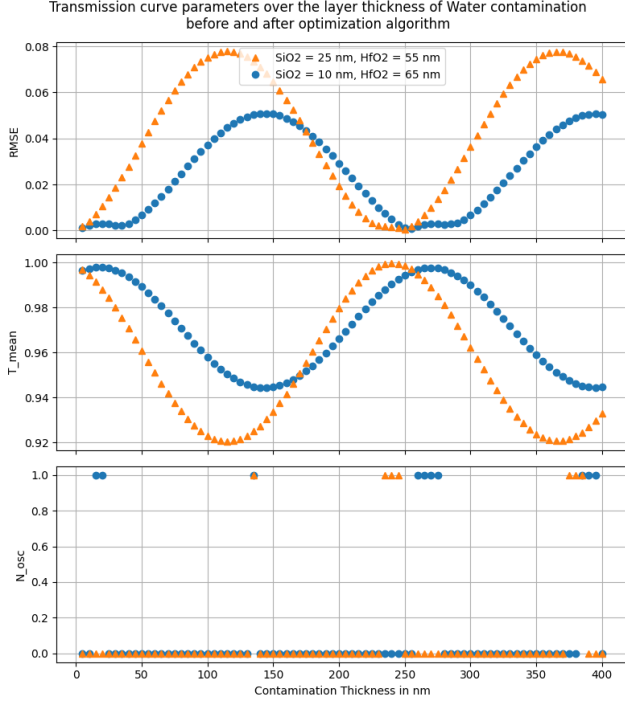


Figure 8: Parameters of the transmission curve at the photosensitive region over the layer thicknesses of different contamination materials for the layer thicknesses of the SiO_2 and HfO_2 layers before and after the optimization algorithm, for the broadband example mission. The optimization algorithm was first applied for all contaminants and then excluding Carbon.



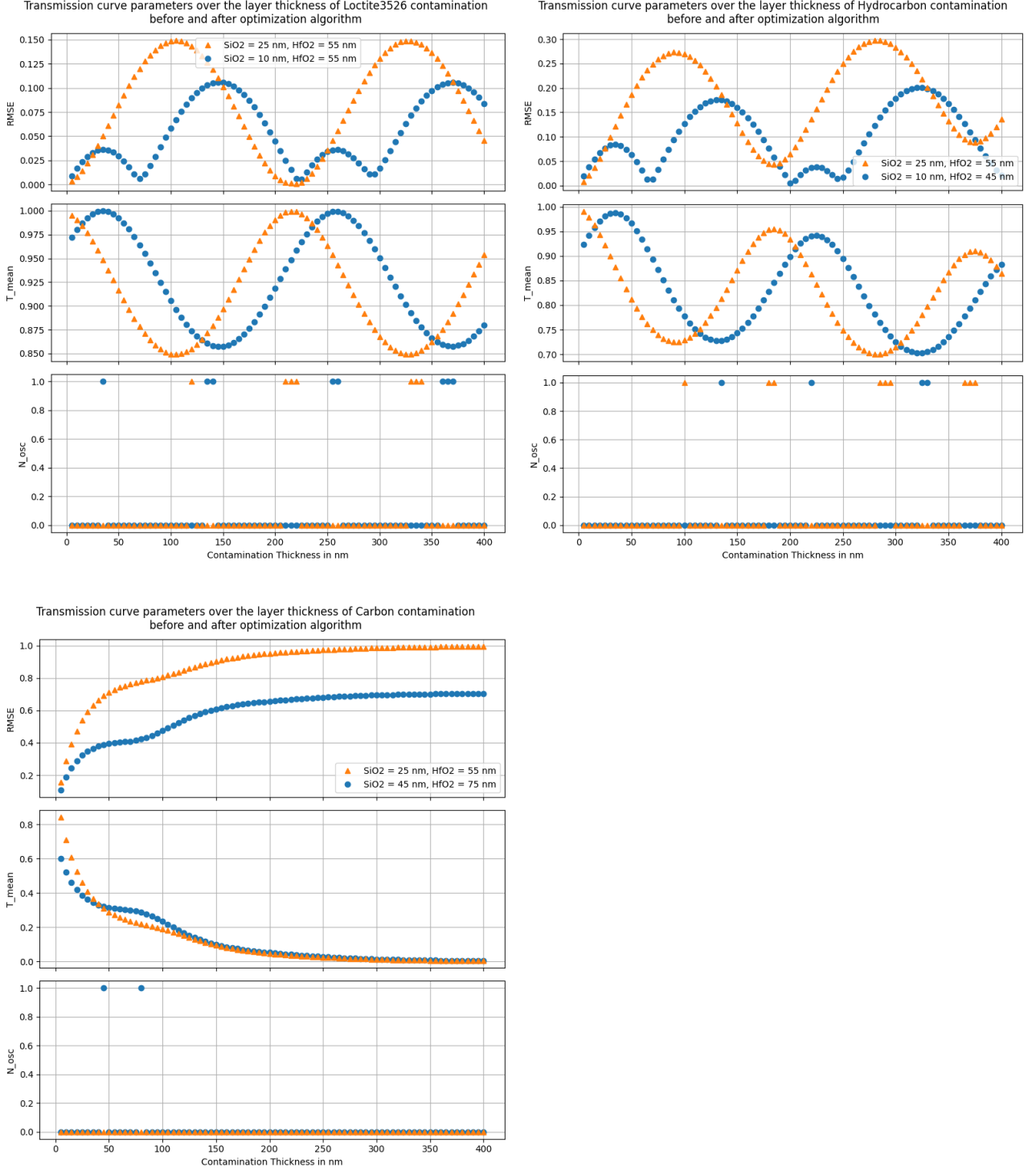


Figure 9: Parameters of the transmission curve at the photosensitive region over the layer thicknesses of different contamination materials for the layer thicknesses of the SiO₂ and HfO₂ layers before and after the optimization algorithm, for the medium-band example mission.

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