Fraunhofer IOF

Characterization of Contamination Induced Straylight (CoCis)

ESR – Executive Summary Report

Doc.-No.:	CoCis-IOF-ESR-24-10-30
Issue:	1.0
Date:	30.10.2024

prepared:	T. Herffurth	date/ signature	
checked:	N. Felde	date/ signature	
	S. Fray	date/ signature	

Distribution Record

	Issue						
	1.0						
INTERNAL:							
IOF intern	C						
EXTERNAL:							
OHB	C						
ESA	C						
Legend *U: updated pages only* *C: complete document*	10/24						

Change Record

Issue	Date	Authorization	Description of Change	Pages
1.0	30.10.24	See cover page	Initial Issue	13

Content

Distribution Record ... 2
Change Record ... 2
Content ... 3
1 Scope ... 3
2 Introduction ... 4
3 Definitions & Methods ... 4
4 Sample Preparation ... 5
5 Measurement Reults ... 5
5.1 PAC analysis ... 5
5.2 BRDF measurement results PAC contamination ... 6
5.2.1 Wavelength scaling of PAC induced scattering ... 7
5.3 MOC analysis ... 7
6 Modelling Results ... 8
6.1 Modelling of scattering induced by PAC ... 8
6.2 Modelling of scattering induced by MOC ... 10
7 Raytracing and scattering simulation at System level ... 11
7.1 General remarks ... 11
7.2 Modelling results at system level (Example) ... 11
8 Summary ... 12
9 References ... 13

1 SCOPE

This document is the “Executive Summary Report” (ESR) a deliverable of the project “Characterization of Contamination Induced Straylight”. The document contains a brief summary of the work done and the results obtained regarding measurement, analysis, and modelling.

2 INTRODUCTION

One of the driving requirements in optical space instrumentation is suppression of straylight. With state-of-the-art polishing techniques [AD1] roughness induced straylight is well controlled and straylight induced by contamination is becoming one of the main contributors to the straylight performance. It is therefore important to rely on representative models for the prediction of contamination induced straylight.

Therefore, the objectives of the activity summarized in this document had been the following:

- Generating practically relevant samples for PAC and MOC on optical surfaces with known/quantified amounts of contamination
- Performing Bidirectional Scatter Distribution Function (BSDF) measurements in transmission and reflection on contaminated samples at wavelengths ranging from ultraviolet to infrared.
- Correlating the contamination and scattering distributions as base for the derivation of scatter models
- Derive guidelines for the modelling and the evaluation of contamination induced straylight in a space project environments

This document provides a brief summary of the designs of the experiments and samples, of the experimental and modelling results for PAC and MOC contamination, as well as of the application of the obtained results for the modelling on system level.

3 DEFINITIONS & METHODS

The basic geometry for the definitions of the scattered and the specular beam directions used in this document to describe angles resolved scattering distributions is shown in the following figure:

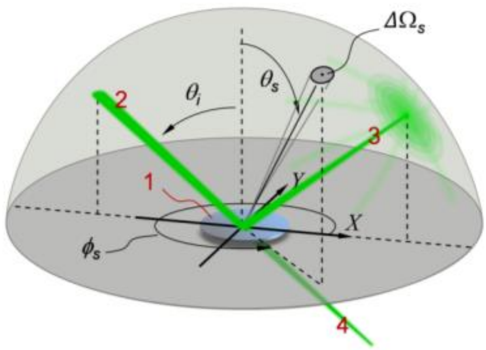


Figure 1: Basic geometry conventions for light scattering: The sample (1) is illuminated by a beam (2) with the power P_i at an angle of incidence θ_i. The specular reflected beam (3) leaves the sample at $\theta_R = \theta_i$ and with the power P_R. Scattered light containing the power ΔP_s is off-specularly redirected into the solid angle $\Delta\Omega_s$ at the polar and azimuthal scattering angles θ_s and ϕ_s, respectively. The sample coordinates are denoted with X and Y.

Typically, the following quantifiers are widely applied to describe angle resolving light scattering: Bi-directional Scattering Distribution Function **BSDF** (ASTM E2387 / SEMI ME1392):

$$BSDF(\varphi_s, \Theta_s) = \frac{\Delta P_s(\varphi_s, \Theta_s)}{P_i \cdot \Delta\Omega_s \cdot cos\Theta_s}$$

Angle Resolved Scattering **ARS**: (ISO 19986:2020) can be calculated from BSDF or vice versa by $ARS(\varphi_s, \Theta_s) = BSDF(\varphi_s, \Theta_s)cos\theta_s$. To show the low scattering levels of the samples discussed in this document ARS will be applied since it reduces the potential of misinterpretation of noise influenced scattering distributions due to the divergence of BSDF at increasing scattering angles.

In advance of the measurement of contamination induced scattering the question how to measure and describe the scattering of an extended surface contaminated with particles of random dimensions and random localization had to be solved. Also the influence the illumination spot diameter on the scattering from singular small features has to be excluded to provide comparable universal results. In the scope of this activity two different random sampling approaches for the measurement position have been evaluated and applied by the partners Fraunhofer IOF and OHB which rely on averaging.

4 SAMPLE PREPARATION

The overall task had several requirements regarding the collection of practically relevant contamination, sample design and sample types, light scattering measurements as well as other analysis methods.

To collect representative particle fall out of different contamination levels in different clean room environments, 22 sample carriers have been prepared. These carriers have been equipped with at least two samples: plane surfaces of Silicon and KG5 glass. Thereby, Si is a mirror like surface that becomes transparent in the near infrared spectral region, whereas KG5 is a (near-) infrared (heat) absorbing glass that becomes transparent in the visible spectral region. Moreover, both sample types were prepared by super-polishing to minimize the roughness induced light scattering of the clean surfaces.

In total, 17 PAC sample carriers have been exposed at 4 different participants in 3 different clean room classes (ISO 5, 7, and 8) from 7 days up to 397 days in a horizontal orientation.

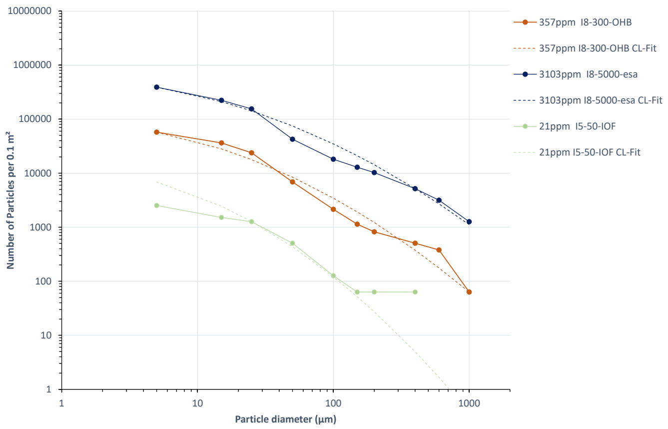
Four sample sets were dedicated to the investigation of MOC induced light scattering. Therefore, the same sample types (Si and KG5) have been used. Further 2” Si wafers were also contaminated in addition to the regular sample sets.

The sample sets were contaminated with epoxy adhesive (EC2216) and silicone rubber (Elastosil RT745) at esa ESTEC, each to two envisaged contamination levels of 2.5e-7 g/cm² and 5e-7 g/cm².

5 MEASUREMENT RESULTS

5.1 PAC analysis

Following the exposure, the accumulated PAC was evaluated using microscopy resulting in values between 3 ppm and 3103 ppm. Moreover, the PAC distribution histogram was evaluated and a fit to a typical cleanliness level distribution (MIL-STD-1246C) was performed. Using the parameters CL for cleanliness level and s for the slope of the distribution in loglog-scale, Figure 2 shows exemplary fitting results.



Sample	CL	s
I5-50-IOF	720	0.5
I8-300-OHB	5829	0.35
I8-5000-esa	24118	0.30

Figure 2: Diagram showing exemplary PAC distributions with corresponding determined CL-fits and Parameters

In the scope of the PAC experiments and analysis, further influences have been analyzed: influence of sample shipping, exposure location close to activity, and cleaning.

Regarding the exposure location no significant trend was observed for the CL and s parameters was observed. However, for the samples exposed in ISO5 clean rooms – that also correspond to low contamination levels – a higher variety of the cleanliness slope was observed (0.24 to 0.63), whereas for higher contamination levels the parameters are primarily between 0.3 and 0.4.

5.2 BRDF measurement results PAC contamination

The following diagrams show the determined average ARS measurements of all sample sets at an angle of incidence of 6°. The Silicon wafers have been characterized at 523 nm and the KG5 glass samples at 1064 nm, respectively. The corresponding PAC levels are indicated by the saturation of the curves and given in the curve labels. In addition to the averaged curves, a representative measurement at a position without contamination is given.

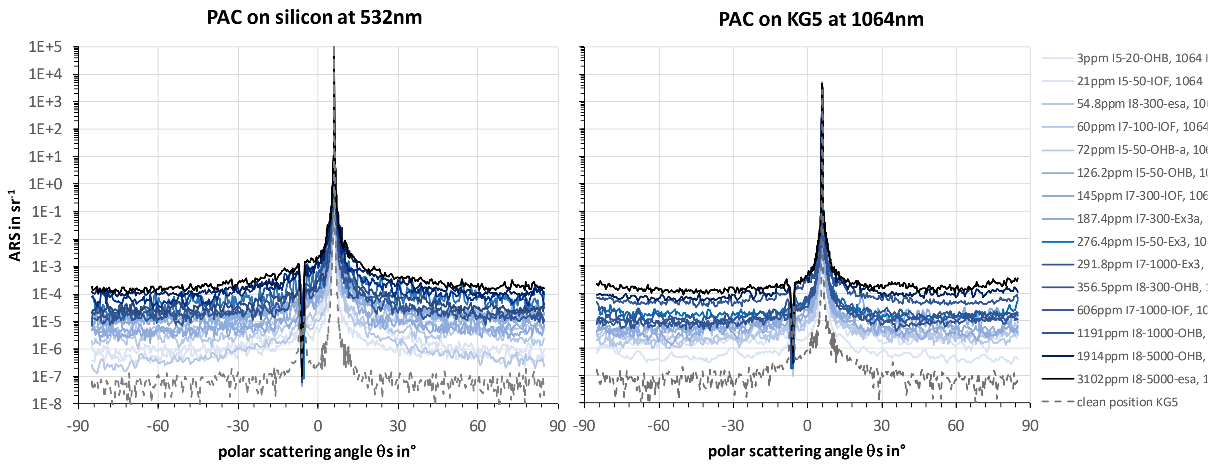


Figure 3: Diagram showing the averaged ARS of the Si-Wafer samples, measured at 532 nm (left); and the KG5 samples measured at 1064 nm (right).

The general trend of increasing ARS according to PAC level is visible for both sample types. However, presumably due to stochastic differences for low contaminated samples, deviations from this trend are observable (e.g. I5-50-IOF vs I5-20-OHB, KG5 samples). Nevertheless, all averaged ARS curves are significantly above the ARS of the clean position without contamination, even for the low contamination levels. Between the contaminated Si and KG5 samples differences in the general slope of the ARS can be observed in particular for higher contamination levels

5.2.1 Wavelength scaling of PAC induced scattering

The Si wafers of four sample sets have been measured at 325 nm, 405 nm, 532 nm, 633 nm, and 1064 nm. These results reveal only minor wavelength related variations in the determined scattering distributions, especially no systematic relations. The reason for the absence of the wavelength scaling is the dominance in the averaged curves of particles much bigger than the wavelength which should not show significant wavelength scaling form a theoretical perspective.

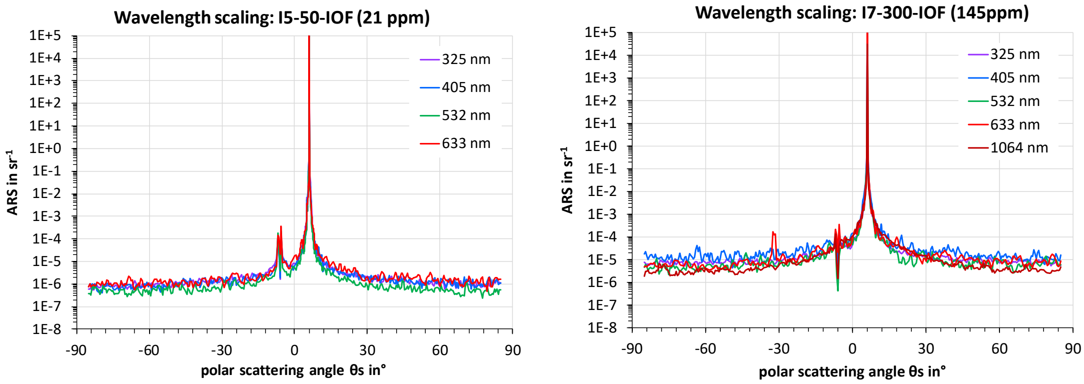


Figure 4: Light scattering from PAC on Si samples measured at 325 nm, 405 nm, 532 nm, and 633 nm (weighted averages).

5.3 MOC analysis

The MOC contaminated samples were investigated using ellipsometry and atomic force microscopy (AFM) to measure the MOC density, MOC thin film thickness, MOC induced changes of the surface roughness, as well as the droplet geometry for the case of droplet like MOC.

Figure 5 summarizes topography data from different positions on the sample surfaces together with the corresponding scattering mappings. Although for the sample EC2216 Low Level on Si shows a quite low and homogeneous scattering over almost the entire surface, the corresponding topography data reveals an increasing roughness towards the sample center. Corresponding Ellipsometry measurement in the sample center and in a distance of 18 mm from the sample center revealed a film thickness of about 2.9 nm and 1 nm, respectively. On the EC2216 High Level sample the MOC in the topography data can be clearly identified as droplets with changing size according to the distance to the sample center.

Figure 6 shows exemplary effects of the MOC contamination on the angle resolved scattering distributions as function if the illumination position that are indicated in the scattering mappings. This droplet like MOC (sample M-HLEC2216-SiA) can cause tremendous increase of the scattering of several orders of magnitude. Moreover, significant alteration of the slope of the ARS might be induced depending on the droplet size.

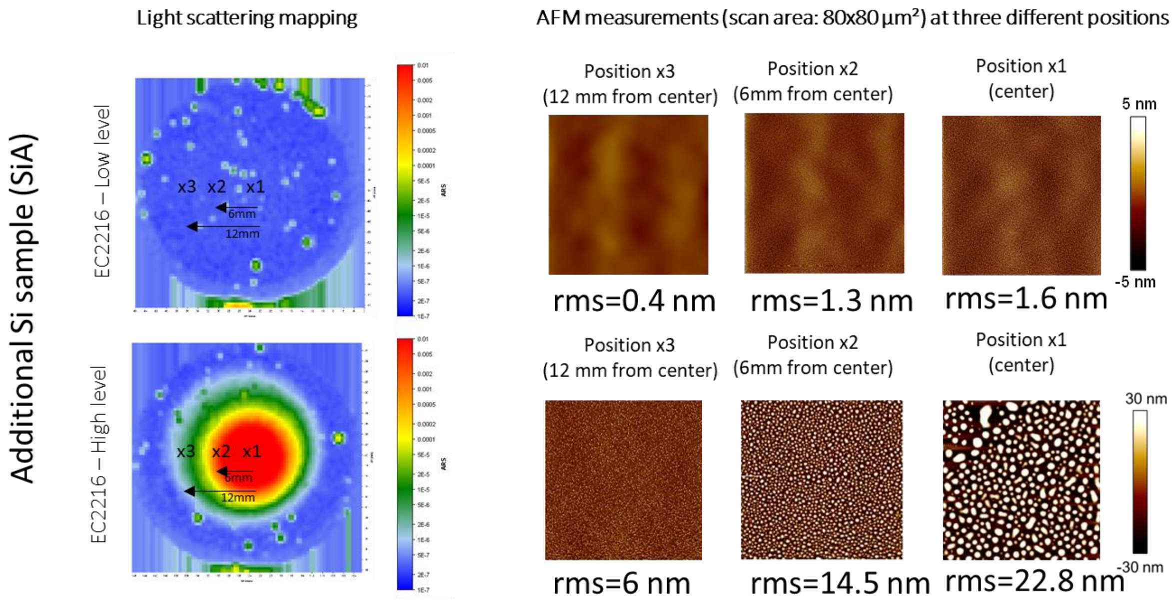


Figure 5: Scattering mappings (532 nm Si samples, 1064 nm for KG5 sample) as well as corresponding topography and roughness data obtained with AFM (80x80 µm² scan area) at different sample positions.

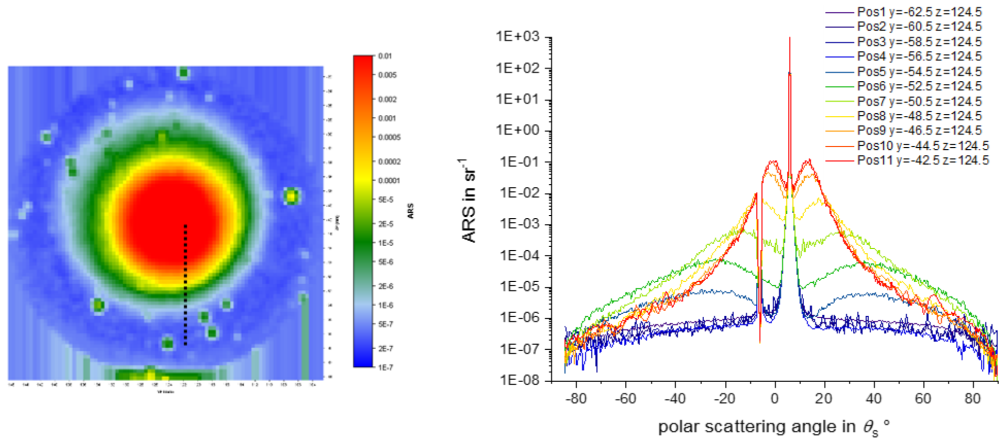


Figure 6: Mapping and angle resolved scattering of M-HL-EC2216-SiA sample at 532 nm.

In contrast, MOC formed as thin films did only cause a small increase of the overall scattering level almost not distinguishable from that of a the clean surface.

6 MODELLING RESULTS

6.1 Modelling of scattering induced by PAC

In the scope of this project the scattering from contamination is investigated in stochastic sense due to the random nature of the topic. It is not claimed to provide exact solutions for the scattering of single particles.

Consequently, the model is based on spherical particles excluding the actual particle form with the same refractive index for all particles (dispersion of particle refractive index is included).

The calculations were performed using the ScatMech library [SCATMECH] provided by NIST either with the MIST [MIST] (MS Windows Executable) or the Python interface [pyScatmech2020]. Therein, the model **Mie scattering with double interaction** [SCATMECH,MIST] that calculates the scattering of a particle using the Mie theory with the surface acting as mirror (or window) was applied.

Using the following modelling procedure almost all effects of the measured curves can be described. These are: Wavelength scaling, PAC scaling, effects of transmitting samples, material effects of the underlying surface, changes in particle distributions after cleaning.

1) The scattering of single particles of defined diameters and refractive indices on surfaces is calculated using the Mie double interaction model for a given wavelength.
2) A weighted sum according to the particle distribution on the actual contaminated surfaces is calculated.

The following diagrams show the measured scattering curve of different Si and KG5-samples at 532 nm and 1064 nm, respectively, together with the corresponding simulated curves, calculated according to the implemented scattering model.

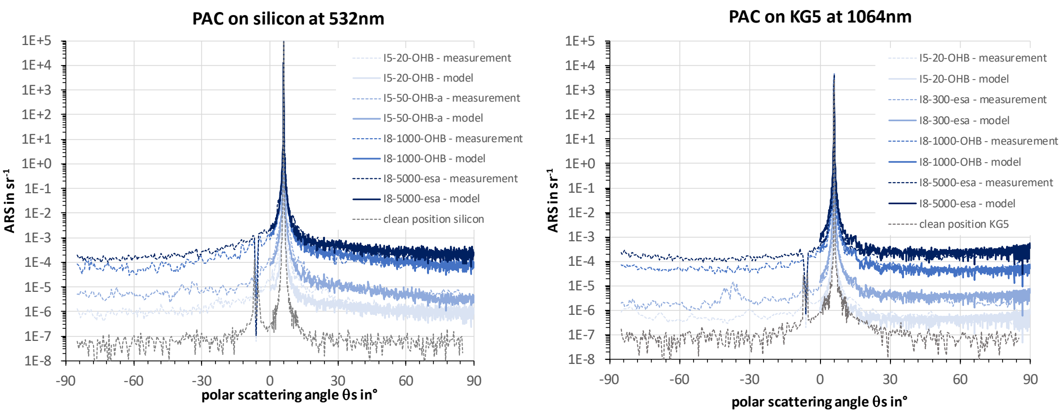


Figure 7: Modeling of ARS from PAC for different Si-samples at 532 nm and KG5-samples at 1064 nm.

The results show good aggrement of the model with the corresponding measurement curves at different ppm-levels. In case of the very low ppm levels, small adaptions in the underlying CL-fit were necessary in order to achieve a better agreement with the measurment. This is presumably due to stochastic effects (for low contamination levels the specifics of single particles have a high relevance for the averaged measurements as well as for the modelling)

Because of the additive nature of the investigated model the scaling according to PAC is linearly if the ratio of particles size is not changed (constant cleanliness-slope s). Since many slopes of the samples are between 0.3 and 0.4 the linear scaling for the samples is supported.

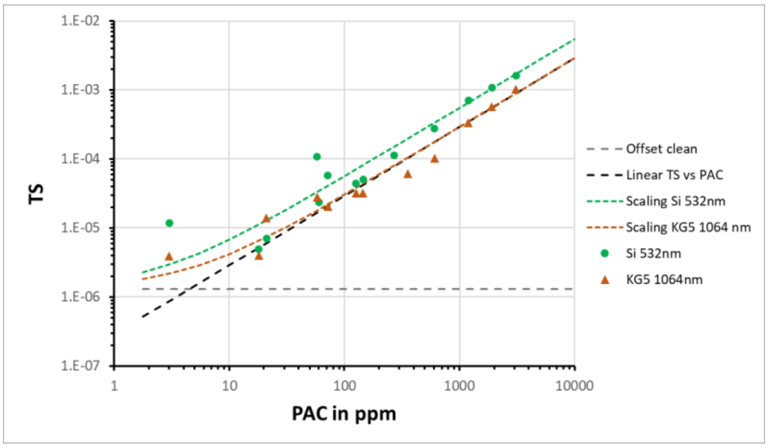
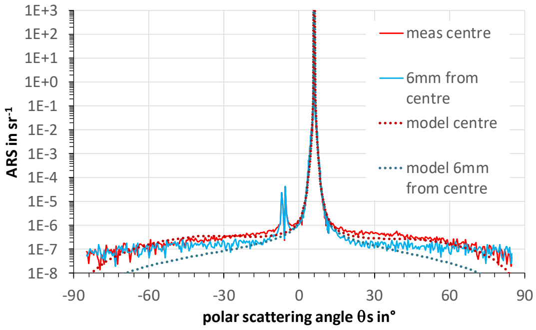


Figure 8: Scaling of the integrated scattering of the averaged experimental scattering data according to the measured PAC for illumination with 532 nm (silicon surface) and 1064 nm (KG5 surfaces).

6.2 Modelling of scattering induced by MOC

Two different MOC characteristics could be generated in the scope of this work: closed thin films with thicknesses of a few nm, slightly increased roughness and scattering close to levels of the clean sample as well as droplets with highly increased scattering. Nevertheless, for both characteristics the light scattering could be modelled using thin film scattering theories for interface roughness [Bousquet1981][Herffurth2014]. For thin film MOC roughness spectra (PSD functions) from topography data determined for the clean samples as well as the contaminated samples could be applied. For droplet MOC the surface roughness spectra with the droplets were determined. By setting thickness of the corresponding “thin film” to about ½ of the maximum droplet height (effective medium) good modelling results have been achieve.



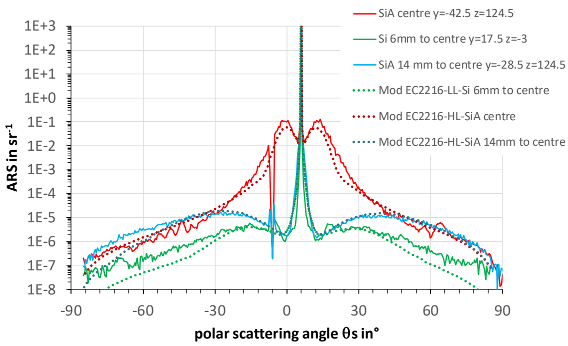


Figure 9: Modeling of scattering from MOC for thin film formation EC-LL-SiA on Silicon at 532 nm (left) and droplet formation (EC-LL Si and EC-HL-SiA) on Silicon at 532 nm (right).

By this approach, a very good agreement regarding the characteristics of the measurements was achieved. In particular the strong increase within +/- 10° towards the specular direction for droplet MOC could be reproduced.

7 RAYTRACING AND SCATTERING SIMULATION AT SYSTEM LEVEL

7.1 General remarks

Raytracing software provides different methods to incorporate contamination induced scattering into a model of an optical system. In the project possibilities for the software FRED have been discussed and its application for an optical is demonstrated using measured and fitted scattering data.

FRED enables particle induced scattering to be implemented for example through importing measured curves, using specific scattering models (Harvey, ABg, …) with (fit) parameters generated from measured curves, applying an implemented MIE based particles scattering model, or by implementing customized scattering models.

This implemented MIE model is quite similar to the double interaction model supposed in this report, beside that phase information and reflectivity is not thoroughly implemented. However, if FRED is using a scattering curve of an interface in transmittance, a scattering angle range of +/-90° is propagated for the BTDF within the volume. Hence, diffraction (and total internal reflection) occurs for the scattered light then passing the second interface and also absorption in the bulk material is added. Therefore, special care is required for the implementation of measured or externally modelled scattering curves into raytracing software since those effects either have to be included or have to be excluded since the raytracing software might add these effects separately.

7.2 Modelling results at system level (Example)

To evaluate the impact of the models at the system level the following optical system consisting of three mirrors, a window and a detector (60x30mm², 0.2mm pixel size) was considered. The optical system has an EFFL of 544.83 mm, a F#=4 and a FOV= ±2.91°. This system consists in an imaging system in the VIS. In the context of this project the system has been evaluated at 0.532 and 1.064 nm.

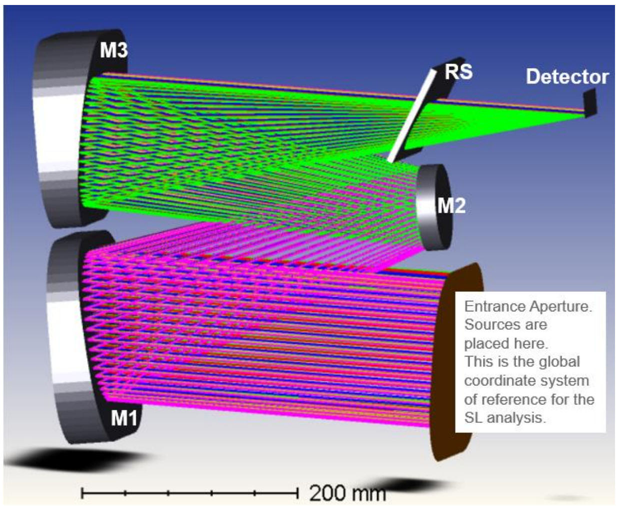


Figure 10: Optical system to evaluate the measured and BSDF model.

The following figures show exemplary results for the nominal and the scattered light on the detector for illuminating this system with a half field light source and a point source.

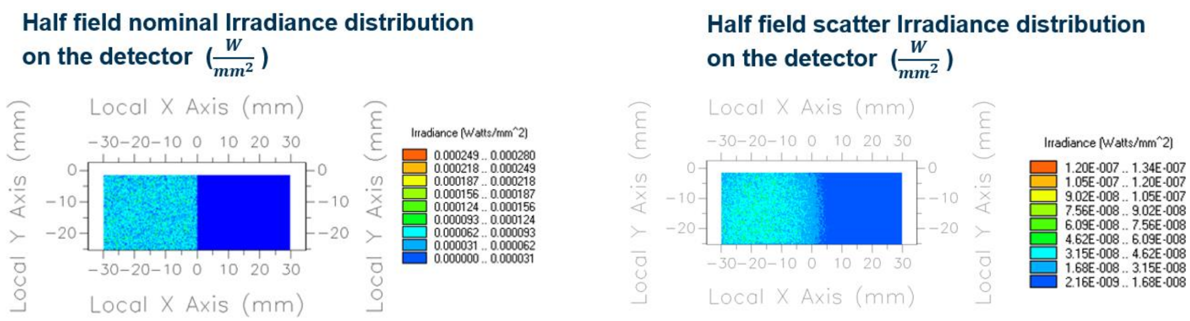


Figure 11: Examples of Irradiance distribution for detector half illumination. On the left can be seen the irradiance distribution of the nominal light. On the right we can see the irradiance distribution of the scatter light on the detector using BSDF measured data.

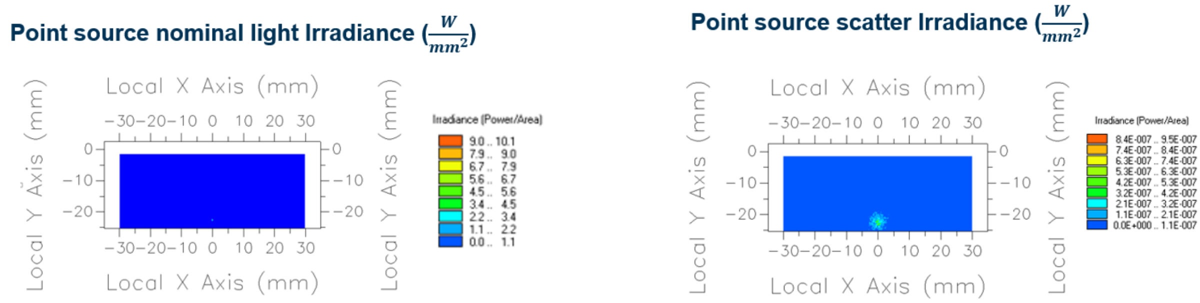


Figure 12: Examples of Irradiance distribution for punctual image on the detector. On the left we can see the irradiance distribution of the nominal light. On the right we can see the irradiance distribution of the scatter light on the detector using BSDF measured data.

8 SUMMARY

The project "Characterization of Contamination Induced Straylight (CoCis)" was a comprehensive study that aimed at understanding light scattering induced by particular and molecular organic contamination (PAC&MOC) on optical surfaces and in optical systems. This involved a systematic approach to generate contaminated samples, conduct Bidirectional Scatter Distribution Function (BSDF) measurements at various wavelengths, and correlate contamination with scattering distributions from an experimental and modelling perspective. The primary objective of this research was to develop representative models and method for predicting and budgeting of straylight caused by PAC and MOC.

To generate representative contaminated samples, sample sets including Silicon wafers and KG5 glasses have been prepared. Thereafter, particular contamination was collected through exposure of those samples at different cleanroom classes (ISO 5, 7, and 8) at laboratories of 4 different participants over extended exposure times. This did result in 17 samples sets with contamination levels from 3 ppm to 3100 ppm. For molecular organic contamination 4 sample sets were contaminated with different levels of epoxy adhesive (EC2216) and silicone elastosil (RT745).

To obtain representative angle resolved scattering distributions of these samples, method for area covering measurements were applied resulting in more than 2000 single scattering measurements. The results revealed significant insights into the relationship between contamination levels and light scattering characteristics with the following major results:

- The PAC induced scattering is increasing (almost linear) according to the PAC level
- For superpolished samples even low PAC contamination levels increase the scattering significantly. An Increase of a factor of >1000 was observed for the highest contamination levels.
- The averaged scattering is dominated by particles significantly bigger than the illumination wavelength. Therefore, no significant wavelength scaling was observed.
- Cleaning by clean nitrogen and isopropanol soaked clean room tissue is reducing the PAC. Thereby, the tissue approach was much more efficient.
- The scattering distributions caused by MOC are significantly driven by the properties of the MOC formation. Thin film MOC with thicknesses of a few nm increases the scattering only slightly compared to a clean superpolished surface. MOC that is forming as droplets might cause a tremendous increase of up to 5 decades depending on the droplet dimensions.

With a MIE scattering based model that relies on the interaction of free space spherical particles with the underlying surface, almost all effects of the measured curves for PAC contamination could be described. These are: Wavelength scaling, PAC scaling, effects of transmitting samples, material effects of the underlying surface, changes in particle distributions after cleaning

For the modelling of MOC induced scattering the application of methods to predict thin film scattering have been demonstrated for both, MOC that formed as droplets and as thin films. This model is based on a Raleigh-Rice scattering theory for smooth surface that requires the surface roughness information in form of roughness spectra.

For application of the results in raytracing simulations, the incorporation of results into optical system models using the software FRED was discussed. Thereby, the importance of preprocessing measured data or the derivation of model parameters from measured data to ensure reliable simulation outcome is emphasized.

9 REFERENCES

[Herffurth2014] T. Herffurth, M. Trost, S. Schröder, K. Täschner, H. Bartzsch, P. Frach, A. Duparré, and A. Tünnermann, “Roughness and optical losses of rugate coatings,” Appl. Opt. 53, A351–359 (2014).

[Bousquet1981] P. Bousquet, F. Flory, and P. Roche, “Scattering from multilayer thin films: theory and experiment,” J. Opt. Soc. Am. 71, 1115–1123 (1981).

[MIST] T. A. Germer, “Modeled Integrated Scatter Tool (MIST),” https://pages.nist.gov/ScatterMIST/docs/index.htm

[SCATMECH] T. A. Germer, “SCATMECH: Polarized Light Scattering C++ Class Library,”

[pyScatmech2020] T. A. Germer, “pySCATMECH: a Python interface to the SCATMECH library of scattering codes,” Proceedings of the SPIE, Volume 11485, id. 114850J 12 pp. (2020).