Final Presentation Project CoCiS:
Characterization of Contamination induced Straylight

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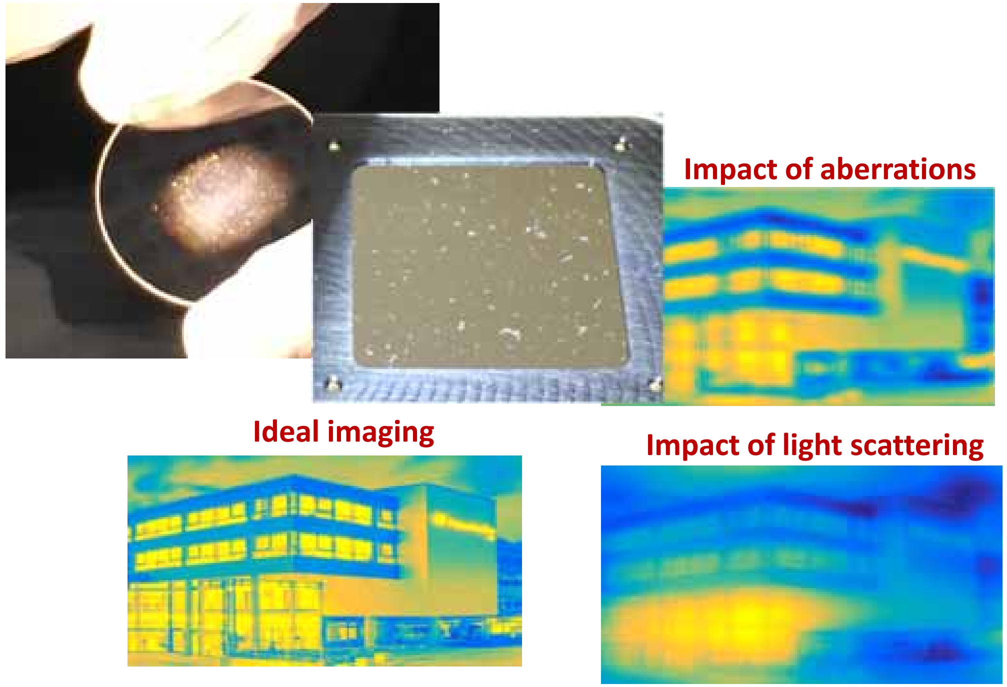
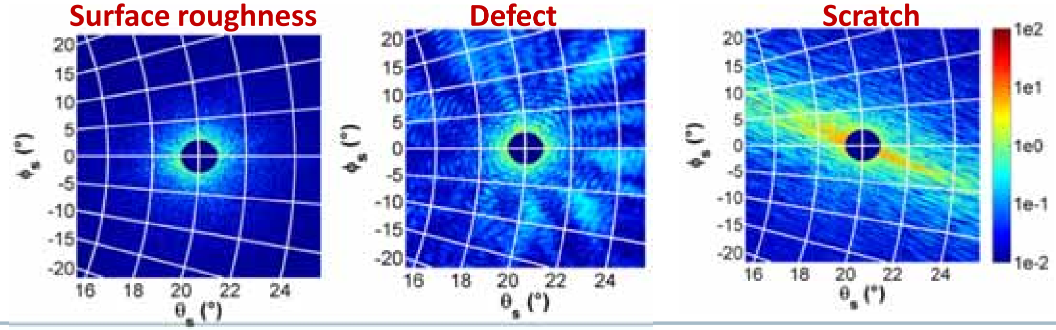
Motivation

- Light scattering unwanted in optical systems:
  - Image degradation, flare
  - Reduced throughput / losses
- Unavoidable origins of scattering
  - Interface roughness, bulk inhomogeneities, …
  - **Defects, particles & MOC**

→ **Scattering measurements & modelling**
  - Quantify scattering distributions
  - Budgeting
  - Performance assessment & prediction (component & system level)





PAC: percent (particle) area coverage
MOC: molecular organic contamination

OHB Fraunhofer IOF

CoCis joint project: Fraunhofer IOF & OHB, (esa)

from experimental fall-out to modelling on system level

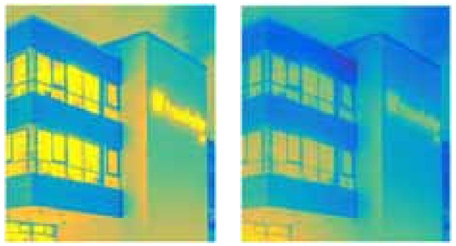
- Goals:
  - Reliable & experimentally verified data & models for contamination induced scattering

  → **Input for raytracing & system modelling**

  → **Input for PAC & MOC budgeting**

- Approach:
  - Collect fall-out:
    PAC (ISO5, ISO7, ISO8) & MOC
  - PAC distribution analysis
  - Scattering measurements from UV to IR
  - Modell development / optimization

Impact of light scattering



imaging by gaussian double lens with 100 ppm (0.1% PAC) contamination

PAC: percent (particle) area coverage
MOC: molecular organic contamination

Agenda / Outline

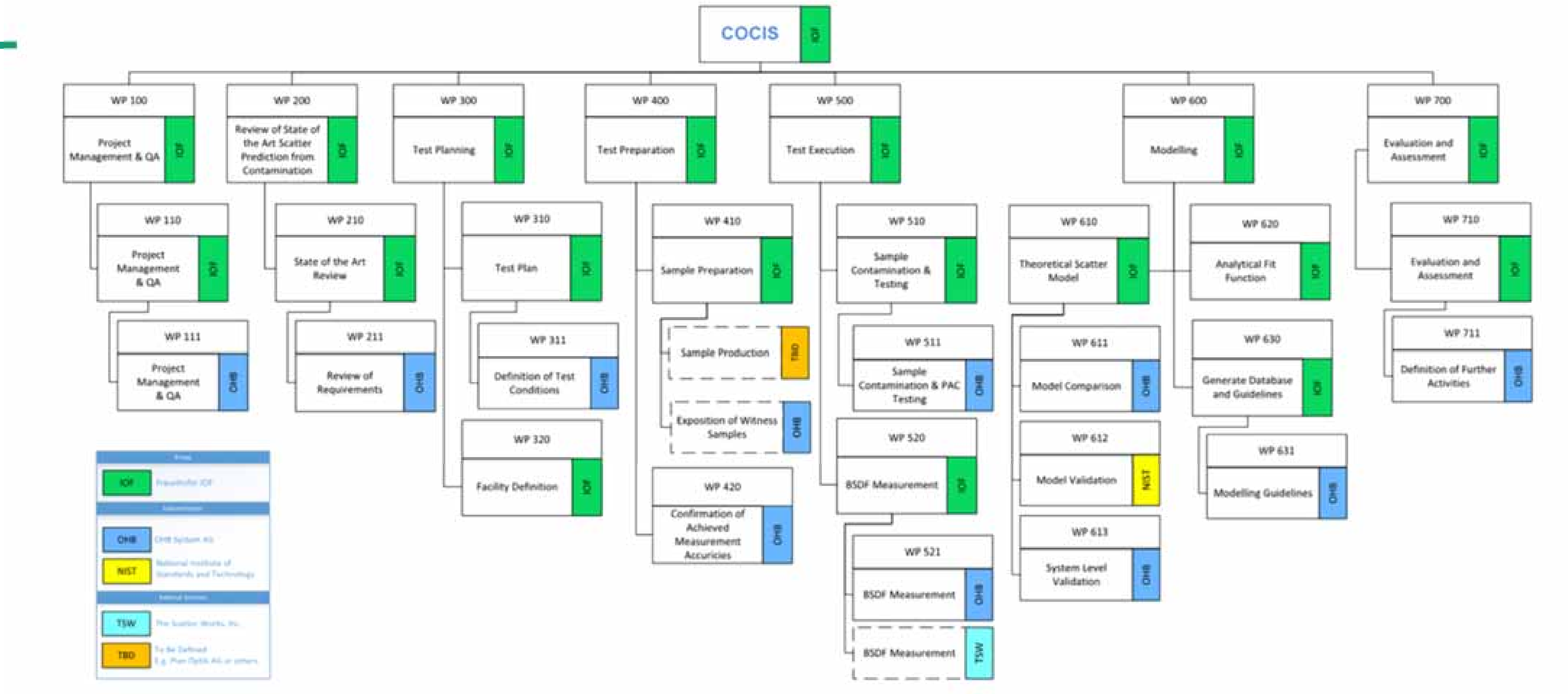
Project CoCiS

Joint project CoCis

- Partners:
  - **Fraunhofer IOF (Jena)**
    - PAC exposure
    - Scattering measurements
    - Additional analysis (topography, microscopy, ellipsometry, …)
    - Model development & analysis
  - **OHB (Munich)**
    - PAC exposure
    - Scattering measurements
    - Additional analysis (PAC-counting, microscopy, FTIR, …)
    - Model development (system level)
  - NIST (USA)
    - Modelling tools
  - esa / ESTEC
    - PAC exposure
    - MOC contamination
  - TSW (The Scatter Works)
    - Scattering measurements
  - Thales
    - PAC exposure

OHB Fraunhofer IOF

Work breakdown structure



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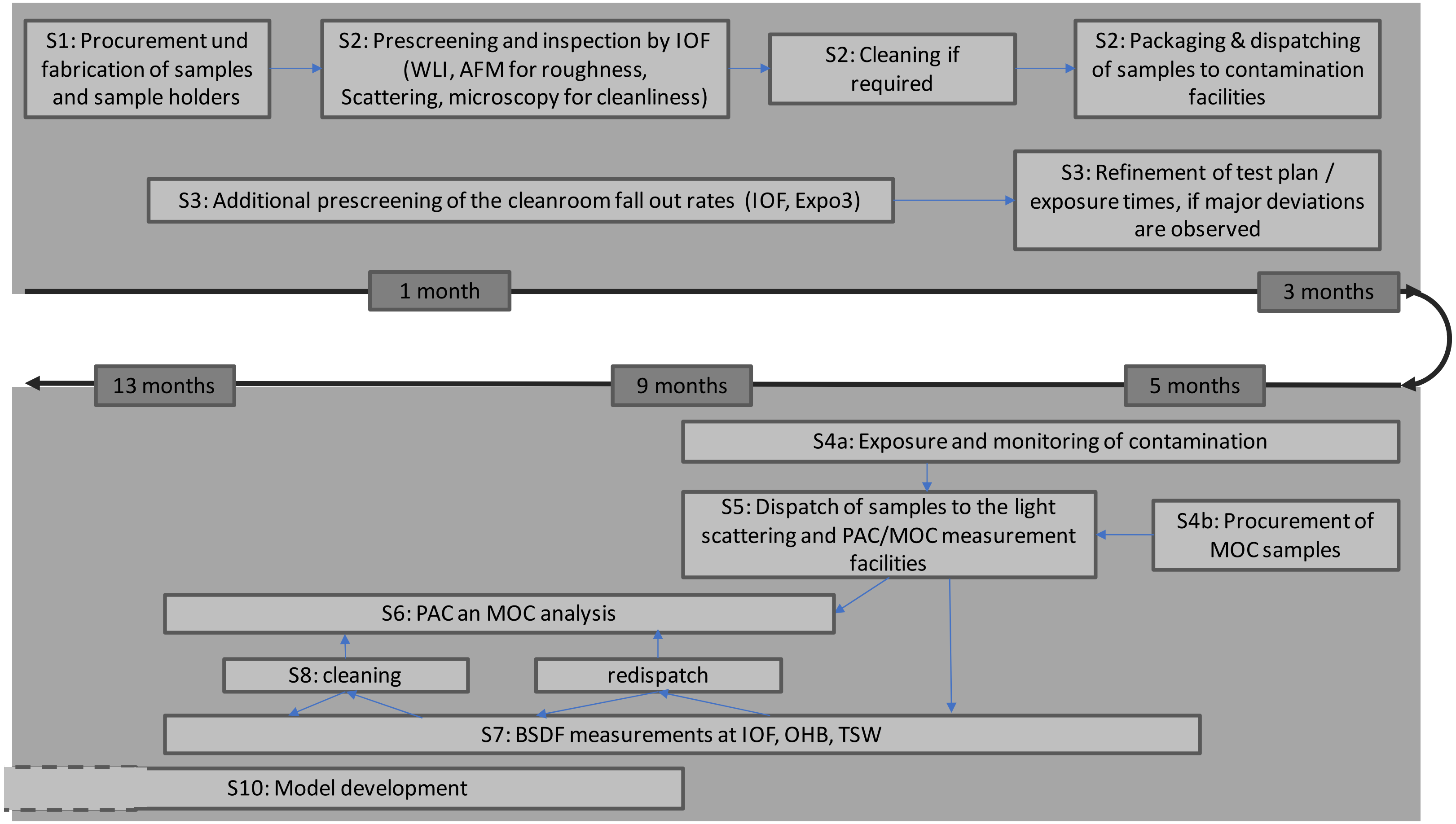
Experimental Work Flow (initial time schedule)



OHB

Fraunhofer IOF

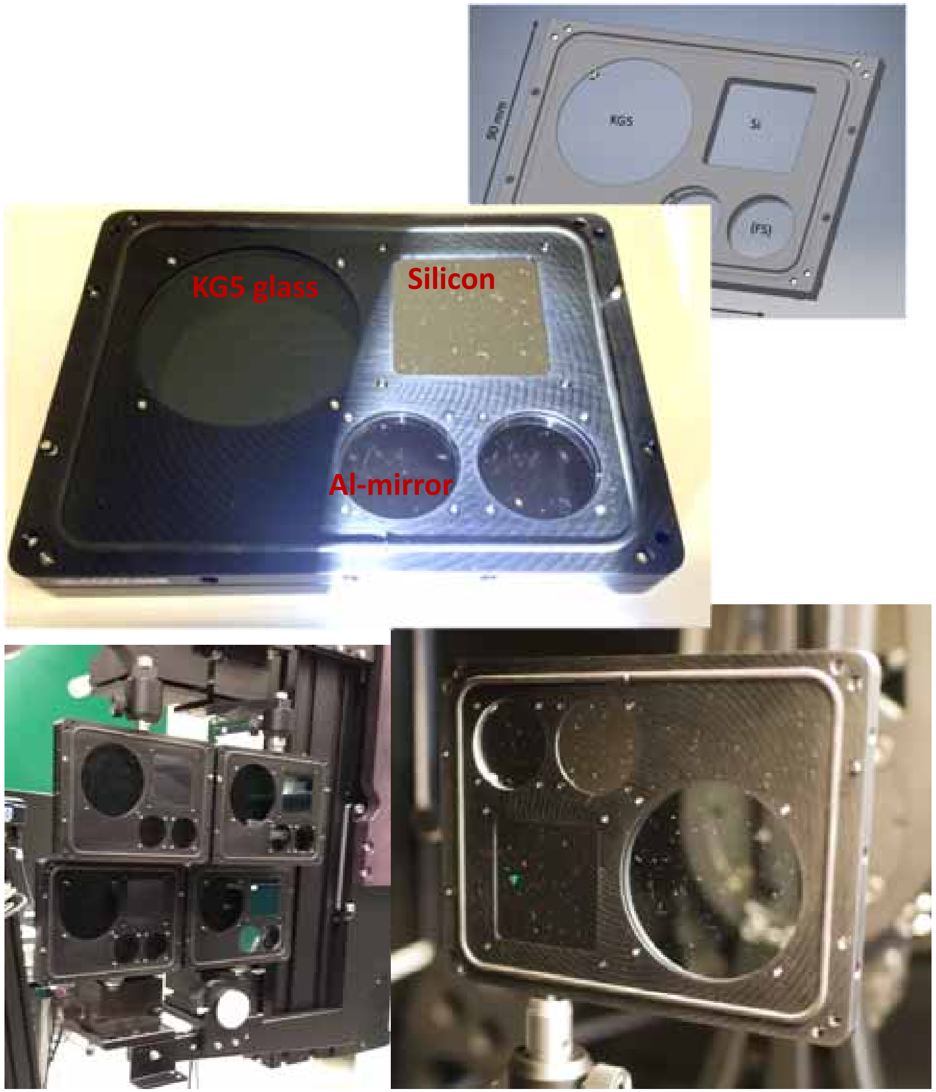
Sample Sets

- Supersmooth Si-Wafer, superpolished KG5 glass
  → low roughness induced scattering (roughness <0.3nm)

- Reflecting/opaque and transmitting samples
  - **Aluminum mirrors** (thin film protected aluminum, reflective from UV/VIS to IR)
  - **Silicon Wafer**
    (reflective in the VIS, transparent in the NIR)
  - **KG5 glass**
    (transparent in the VIS, reflective in the NIR)

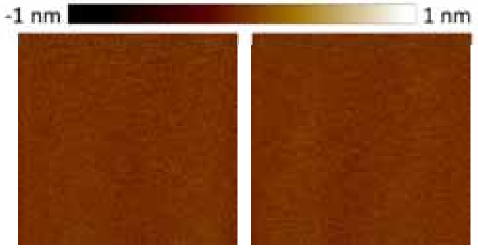
- KG5 also for PAC counting at OHB (transparent sample required)

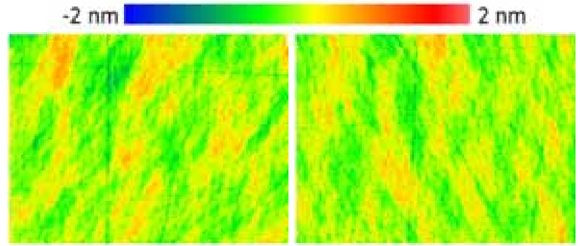
- No disassembly required for mounting in scatterometers

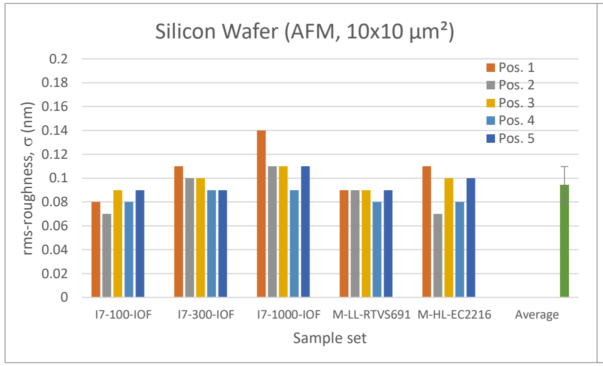


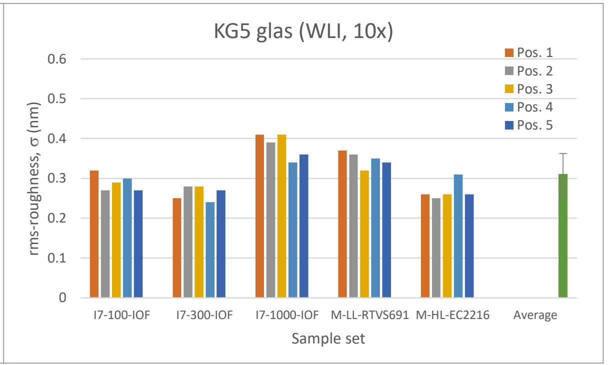
OHB Fraunhofer IOF

Sample Sets – pre-screening

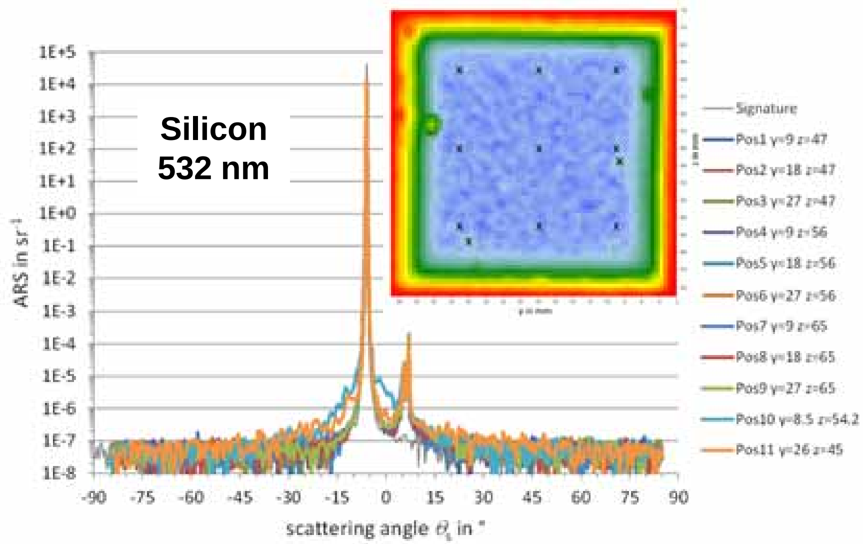


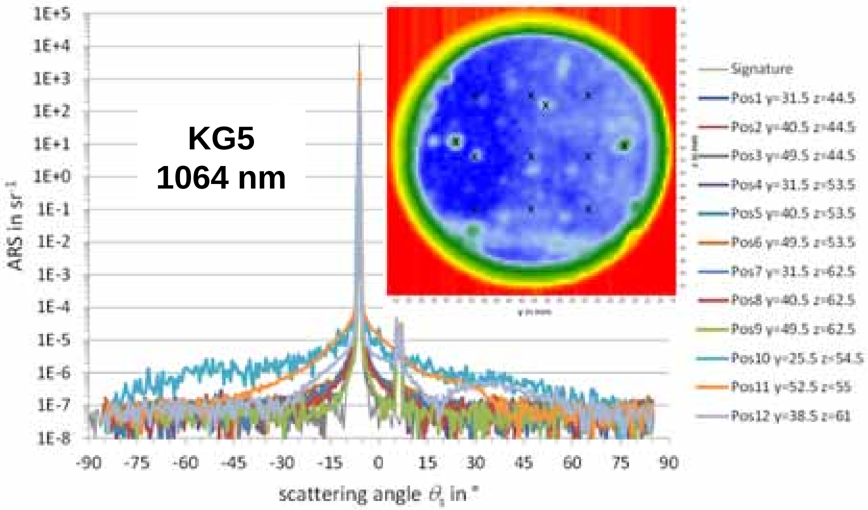






- Roughness and cleanliness cross checks during procurement and assembly
- First scattering measurements of initial state





OHB Fraunhofer IOF

PAC Exposing labs

- Planned ppm levels from 20ppm to 5000ppm

- **ISO 5** clean room available at: OHB, IOF, Thales
- **ISO 7** clean room available at: IOF, Thales
- **ISO 8** clean room available at: OHB, esa, Thales

- Pre-screening results:
  - 1 to <10ppm for Si Wafer initially
  - 50 … 100 ppm for KG5 (defects)

- Pre-test to estimate exposure time:
  <~ 1ppm/day in ISO5; ~10 ppm/day in ISO8

- Continuous monitoring during exposure if available or cross checks on short exposure samples

Envisaged PAC ↓

Number of sample sets + envisaged exposure time

	IOF, OHB, Expo3 ISO 5		IOF, Expo3 ISO 7		OHB, esa ISO 8	
	Exposure time	Sample set	Exposure time	Sample set	Exposure time	Sample set
20 ppm	1 to 2 Months	1x	-		-	
50 ppm	5 Months, 2 Months (activity)	3x +1x close to the activity	-			
100 ppm	-		10 days	1x	-	
300 ppm	-		1 Month, 3 Weeks (activity)	2x +1x close to the activity	5 Days	2x
1000 ppm	-		4 Months	2x	3 Weeks, 2 Weeks (activity)	1x + 1x close to the activity
5000 ppm	-		-		4 Months,	2x
Total		5x		6x		6x

(Original Expo3 disagreed with disclosure → Thales stepped in)

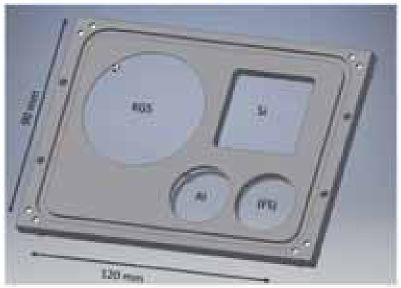
MOC generation

- MOC contamination at dedicated esa/ESTEC facility (M. Helici, H. Fischer)

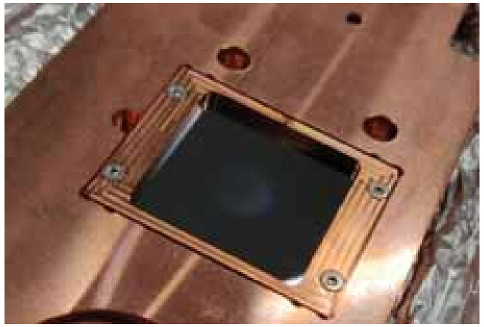
- MOC sample sets: Si, KG5; + ZnS sample for FTIR analysis
- Additionally: 2“ Si Wafers

- Contaminants
  - Epoxy adhesive **EC2216**
  - Silicone Elastosil **RT745**
  - initially planned Dowsil 93-5000 or RTV-S 691
    → problems in generating reasonable MOC

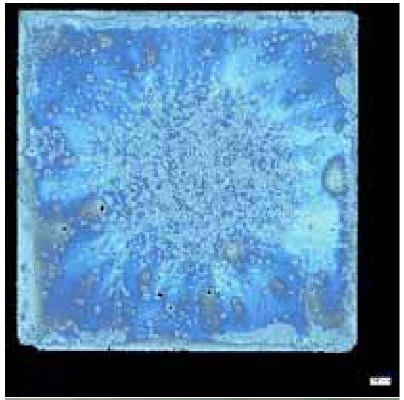
- Envisaged contamination levels:
  250 ng/cm² & **500 ng/cm²**

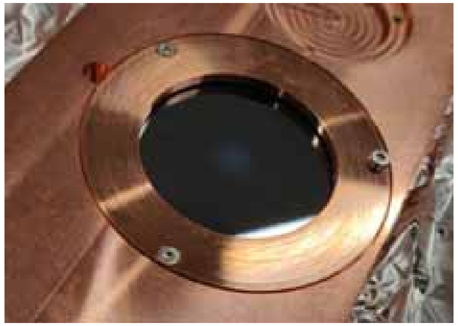


EC2216 on Si



RT745 on Si

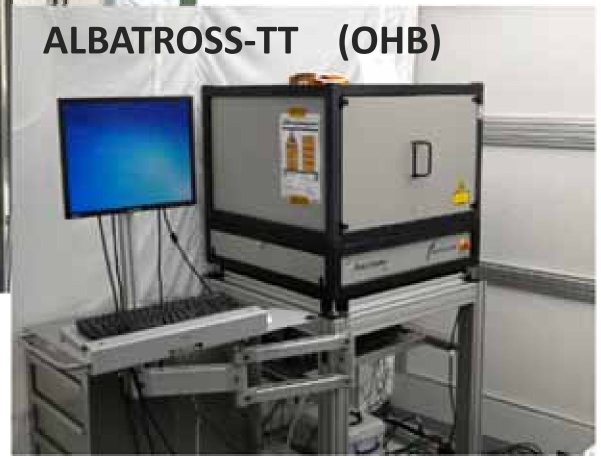




EC2216 on Si

Scattering Labs

- Fraunhofer IOF
  - All sample sets
  - Primarily **532nm & 1064nm**
    (+ 325nm, 405nm, 633nm, 10600nm)
  - > 1000 single BRDF measurements
- OHB
  - 6 sample sets
  - **532nm & 1064nm**
  - > 610 single BRDF measurements
- TSW (The Scatter Works)
  - 3 sample sets
  - Cross check measurements at 532 nm
  - Additionally at 1550 nm



CASI (TSW)

Plan

17x PAC sample sets

Identifier		Cl	Goal	Facility	PREESCREENING	4	5	6	7	8	9	10	11	12	13
I5-20-OHB	Si KG5 Al	ISO 5	20 ppm	OHB	in1 (cl1) cl1 (cl1) as	tr in1 pc1 x x	x x x x	x x pc1 sc1	532 1064 tr	sc1 532 532 532					
I5-50-IOF	Si KG5 Al	ISO 5	50 ppm	IOF	in1 (cl1) cl1 (cl1) as x	x x x x	x x x x	x x x x	x x x x	x x x sc1	1064, 325 1064 10600 10600 532+, 640 Near 532 532	tr pc1	tr pc2		
I5-50-OHB	Si KG5	ISO 5	50 ppm	OHB	in1 (cl1) cl1 as	tr in1 pc1 x x	x x x x	x x x x	x x x x	x x x x	x x	pc1	tr sc1 532 1064	cl2 sc1 532 1064	tr pc1
I5-50-Ex3	Si KG5	ISO 5	50 ppm	Expo3	in1 (cl1) cl1 as	tr in1 x x	x x x x	x x x x	x x x x	x x x x	x x tr	pc1	tr sc1 532 1064	cl3 sc1 532 1064	tr pc1
I5-50-OHB-a	Si KG5	ISO 5	50 ppm	OHB-activity	in1 (cl1) cl1 as	tr in1 pc1 x x	x x x x	x x pc1 sc1	532 1064 tr	sc1 532 1064		tr tr sc1	532, 1550 532, 1550 tr	tr sc1 532 1064	tr pc1
I7-100-IOF	Si KG5 Al	ISO 7	100 ppm	IOF	to in1 (cl1) cl1 (cl1) as	sc1 sc2 532 1064 532 x x	in2 pc1	sc1 532 532 532		sc1	325	tr pc1			
I7-300-IOF	Si KG5 Al	ISO 7	300 ppm	IOF	to in1 (cl1) cl1 (cl1) as	sc1 sc2 532 1064 532 x x	x x in2 pc1	sc1 532+ 532 532		1064 1064	325 10600 10600 640 Near	tr pc1	tr pc2		
I7-300-Ex3	Si KG5	ISO 7	300 ppm	Expo3	in1 (cl1) cl1 as	tr in1 x x	x x tr	pc1	tr	sc1 532		tr pc1	tr pc2		
I7-300-Ex3-a	Si KG5	ISO 7	300 ppm	Expo3-activity	in1 (cl1) cl1 as	tr in1 x x	x tr	pc1 sc1	532 1064 532 1064 tr	sc1 532 1064		tr tr sc1	532, 1550 532, 1550 tr	tr sc1 532 1064	tr pc1
I8-300-OHB	Si KG5	ISO 8	300 ppm	OHB	in1 (cl1) cl1 as	tr in1 pc1 x pc1	tr tr	pc1 sc1	532 1064 532 1064 tr	sc1 532					
I8-300-esa	Si KG5	ISO 8	300 ppm	esa	in1 (cl1) cl1 as	tr in1 x in2	tr	pc1	tr	sc1 532 1064		in2 pc1 tr pc1	tr pc2		
I7-1000-IOF	Si KG5	ISO 7	1000 ppm	IOF	to in1 (cl1) cl1 as	sc1 sc2 532 1064 x x	x x x x	x x x x	x x x x	x x in2 pc1		tr pc1	tr sc1 532 1064	cl2 sc1 532 1064	tr pc1
I7-1000-Ex3	Si KG5	ISO 7	1000 ppm	Expo3	in1 (cl1) cl1 as	tr in1 x x	x x x x	x x x x	x x x x	x x	tr	pc1	tr sc1 532 1064	cl3 sc1 532 1064	tr pc1
I8-1000-OHB	Si KG5 Al	ISO 8	1000 ppm	OHB	in1 (cl1) cl1 (cl1) as	tr in1 pc1 x x	x	pc1 sc1	532 1064 532 1064 tr	sc1 532+ 532 532 1064	325 10600 10600 640 Near	tr tr sc1	532, 1550 532, 1550 tr	tr sc1 532 1064	tr pc1
I8-1000-esa-a	Si KG5	ISO 8	1000 ppm	esa-activity	in1 (cl1) cl1 as	tr in1 x x	in2 tr	pc1	tr	sc1 532		in2 pc1 tr pc1	tr pc2		
I8-5000-OHB	Si KG5 Al	ISO 8	5000 ppm	OHB	in1 (cl1) cl1 (cl1) as	tr in1 pc1 x x	x x x x	x x x x	x x x x	x x sc1	532 1064 532 1064	pc1	tr sc1 532, 1064 532, 1064 532	325	
I8-5000-esa	Si KG5	ISO 8	5000 ppm	esa	in1 (cl1) cl1 as	tr in1 x x	x x x x	x x x x	x x x x	x x in2 tr		pc1	tr sc1 532		
control	Si KG5				in1 (cl1) cl1 as					sc1 532+ 532 1064, 325 1064	10600 640 Near	tr pc1			

4x MOC sample sets

Identifier		Cl	Goal	Facility	PREESCREENING	4	5	6	7	8	9	10	11	12	13
M-LL-EC2216	Si KG5 ZnS	MOC	low level	EC2216	in1 (cl1) cl1 (cl1) as		tr FTIR	tr x x	x x tr in3	sc1 532 1064	tr FTIR				
M-LL-RTVS691	Si KG5 ZnS	MOC	low level	RTV-S 691	to in1 (cl1) cl1 (cl1) as sc1 sc2	532 1064	tr FTIR	tr x x	x x tr in3	sc1 532 1064	tr FTIR				
M-HL-EC2216	Si KG5 ZnS	MOC	high level	EC2216	to in1 (cl1) cl1 (cl1) as sc1 sc2	532 1064	tr FTIR	tr x x	x x tr in3	sc1 532 1064	tr FTIR				
M-HL-RTVS691	Si KG5 ZnS	MOC	high level	RTV-S 691	in1 (cl1) cl1 (cl1) as		tr FTIR	tr x x	x x tr in3	sc1 532 1064	tr FTIR				

Agenda / Outline

1. Motivation & Goals
2. Project CoCis
    1. Participants
    2. Project plan
3. Definitions & Approaches
4. Experimental results
    1. PAC fall out results
    2. Scattering from PAC
    3. Scattering from MOC
5. Modelling
    1. Scatter modelling from PAC
    2. Scatter modelling from MOC
    3. Modelling on system Level
6. Summary / Conclusions

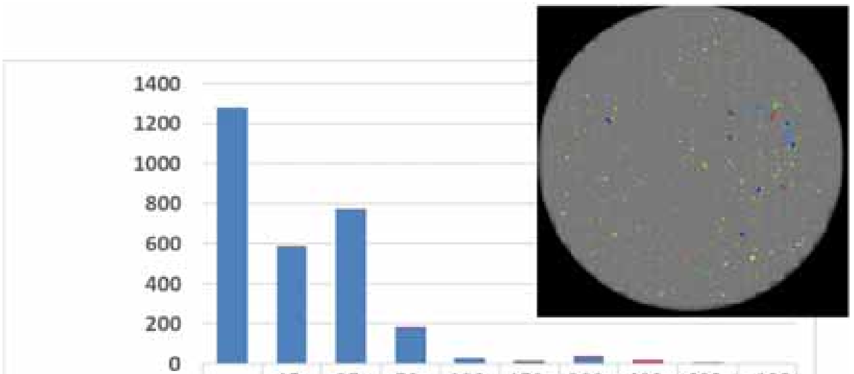
Definitions

OHB Fraunhofer IOF

PAC

- **PAC – percent (particle) area coverage**
  (synonym for particle contamination)
- obscured surface area by particles in ppm
- PAC counting via microscopy (bright field)
  + image processing at OHB

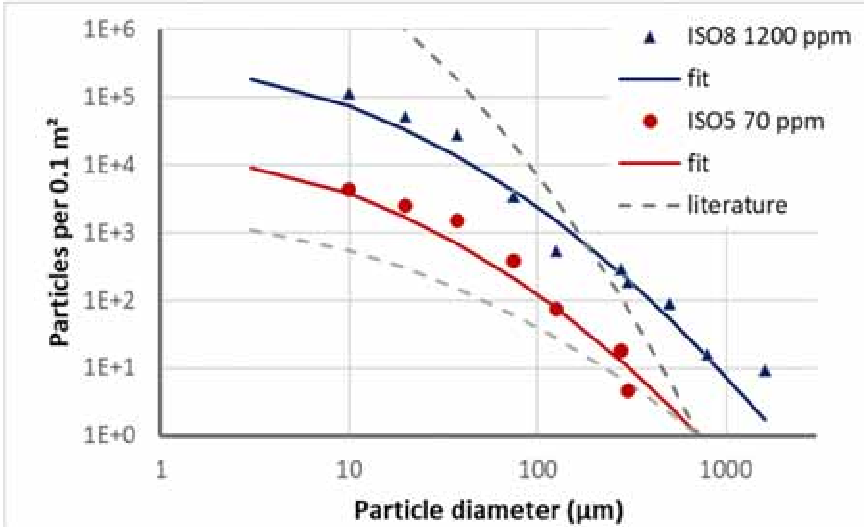
→ PAC level in ppm + histogram



	5-15 B	15-25 C	25-50 D	50-100 E	100-150 F	150-200 G	200-400 H	400-600 I	600-1000 J	>1000 K
Fasern	0	1	4	4	0	3	10	19	4	3
rundl. Partikel	1278	587	773	180	30	13	32	1	3	1

- Often density / frequency / **distribution** described by two parameter function (MIL-STD-1246C):
  CL – Cleanliness level & S - slope

$$N(S, CL, D) = 10^{|S|[\log^2(CL) - \log^2(D)]}$$



- D = minimal particle diameter of the class;
  N = number of particles per 0.1 m²

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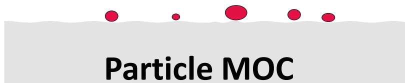
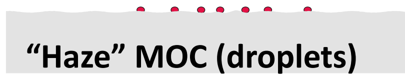
MOC

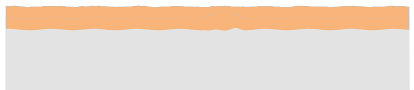
- **MOC – molecular organic contamination**
- Described in mass density in ng/cm²

- Formation: thin film, droplets or particles ?

- Analysis with:
  - FTIR → mass density
    highly averaged, no local resolution
  - **Ellipsometry → optical film thickness**
    locally resolved thin film properties
  - **AFM → topography**
    locally resolved droplet properties







Thin film MOC (nm range)

FTIR: Fourier Transform Infrared Spectroscopy
AFM: Atomic Force Microscopy

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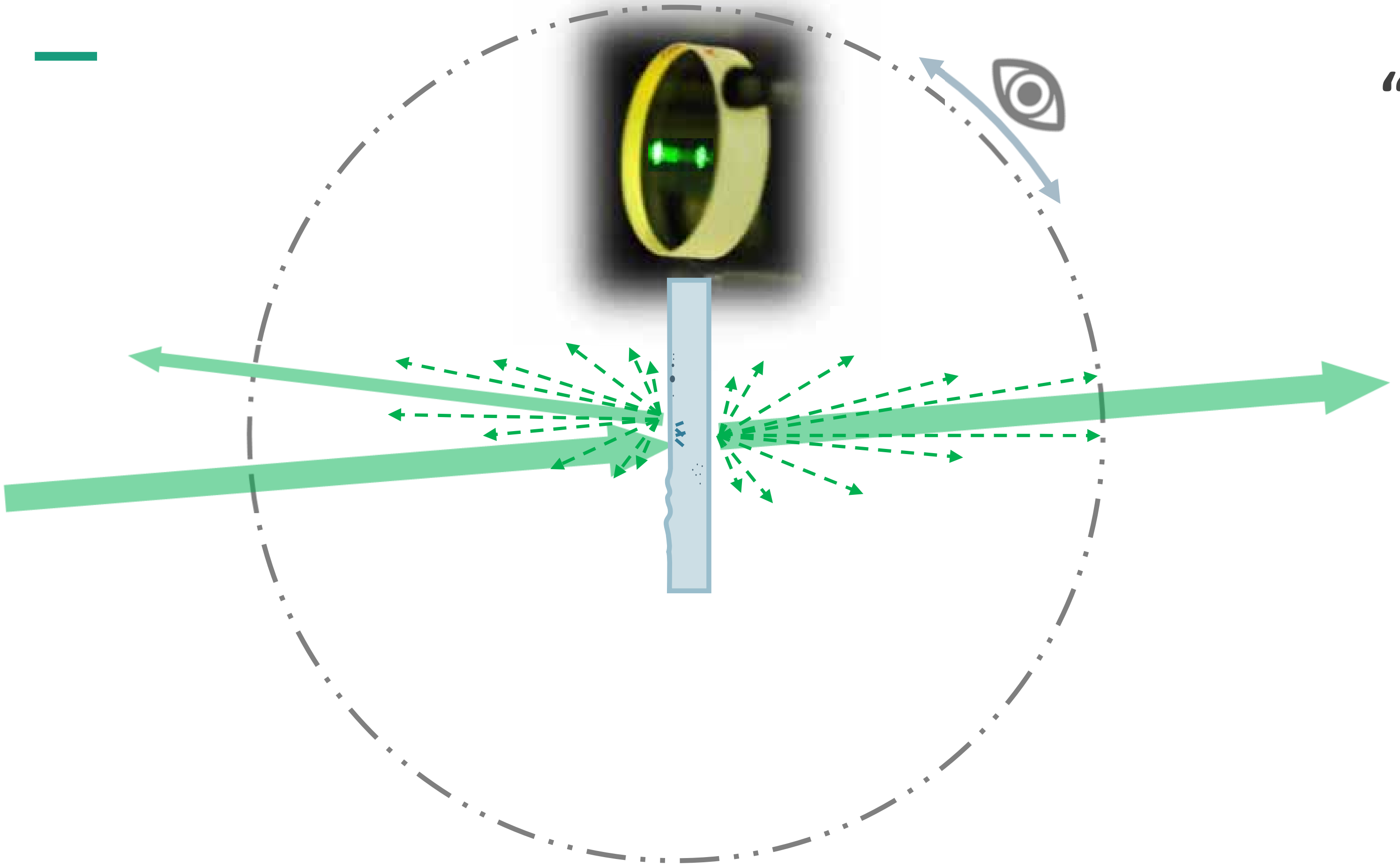
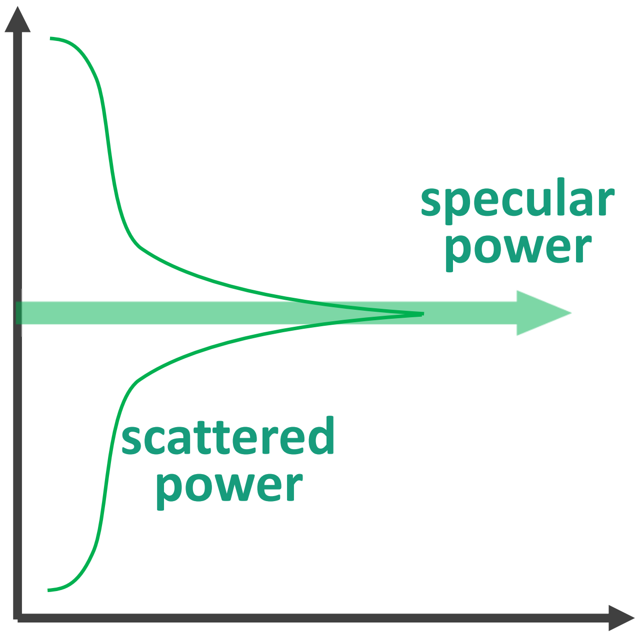
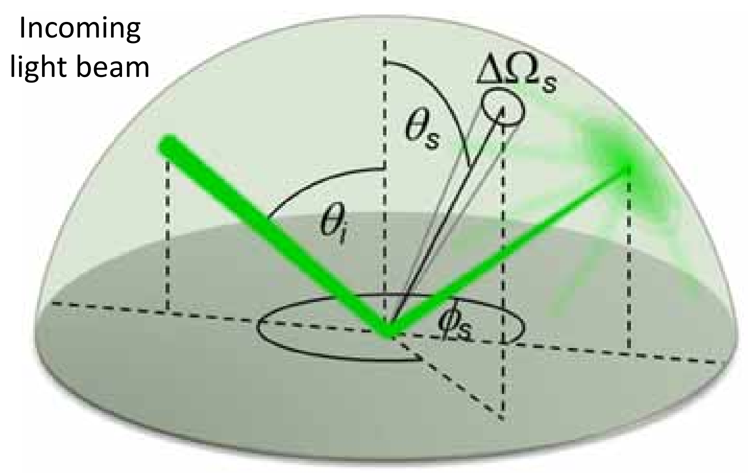
Light scattering





Light scattering quantities



θ_s ... polar scattering angle
φ_s ... azimuthal scatter angle
P_s ... scattered light power
P_i ... incident light power
P_r ... specularly reflected light power
$\Delta\Omega_s$ ... detector solid angle

Angle Resolved Scattering (ISO19986)

$$\mathrm{ARS}(\theta_i, \theta_s, \varphi_s) = \frac{\Delta P_s(\theta_i, \theta_s, \varphi_s)}{\Delta\Omega_s P_i}$$

$$\mathrm{BSDF}(\theta_i, \theta_s, \varphi_s) = \frac{\text{differential radiance}}{\text{differential irradiance}} = \frac{\mathrm{ARS}(\theta_i, \theta_s, \varphi_s)}{\cos\theta_s}$$

- B**R**DF for reflection hemisphere
- B**T**DF for transmission hemisphere

Total scattering (ISO13696)

$$\mathrm{TS} = \int_0^{2\pi} \int_{2°}^{85°} \mathrm{ARS} \sin\theta_s \, d\theta_s d\varphi_s$$

- Scattering loss
- Energy balance: 100% = R + T + A + TS_b + TS_f

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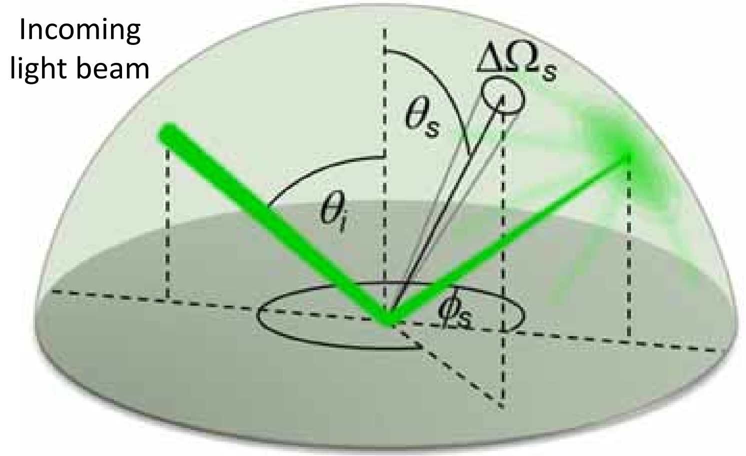
Light scattering quantities



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- Scattering loss
- Energy balance: 100% = R + T + A + TS_b + TS_f

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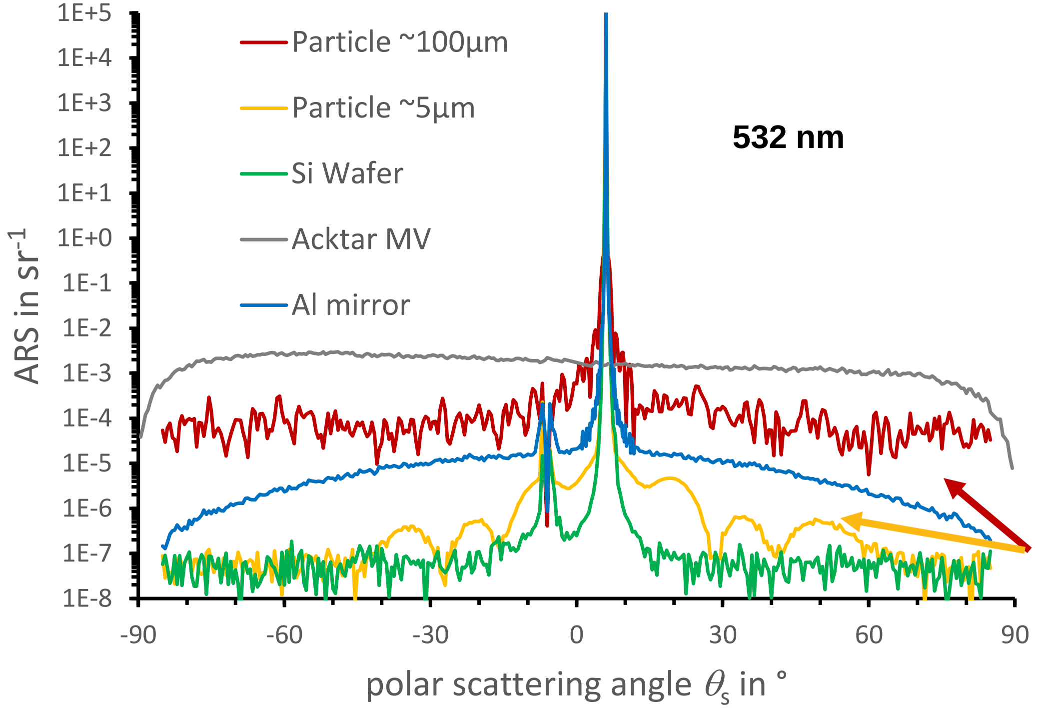
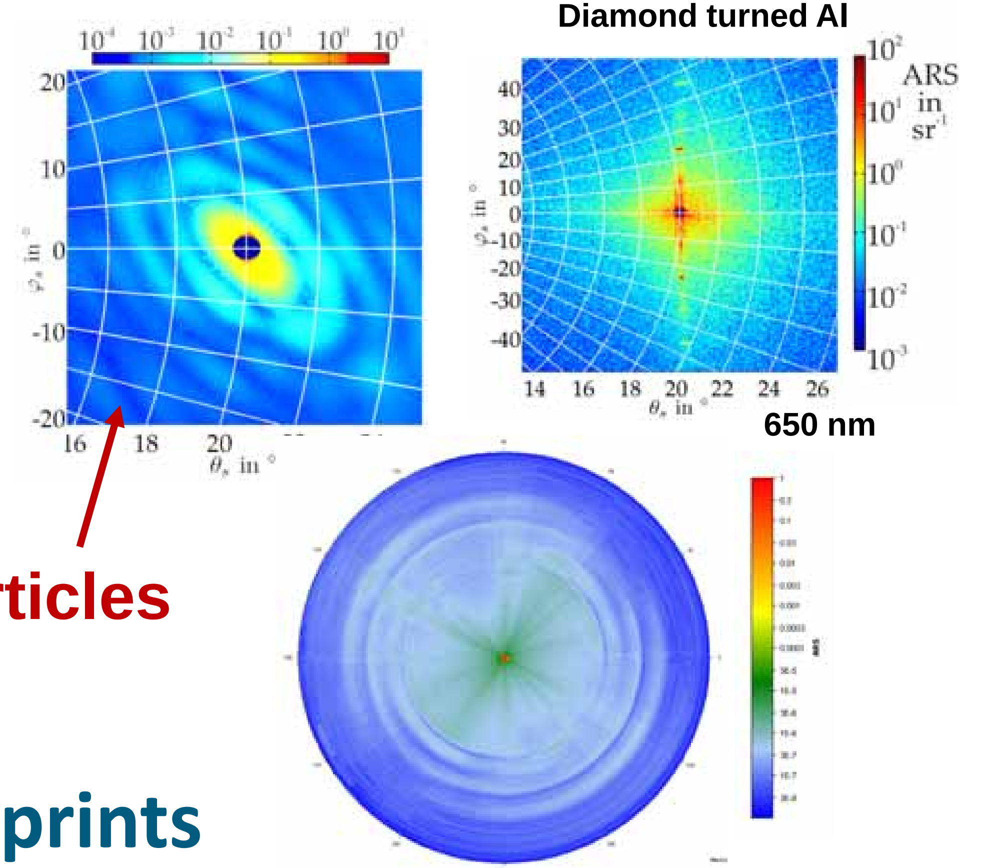
Typical Angle Resolved Scattering distributions

"2D in plane of incidence"



"3D scattering"



Particles

→ Scattering Footprints

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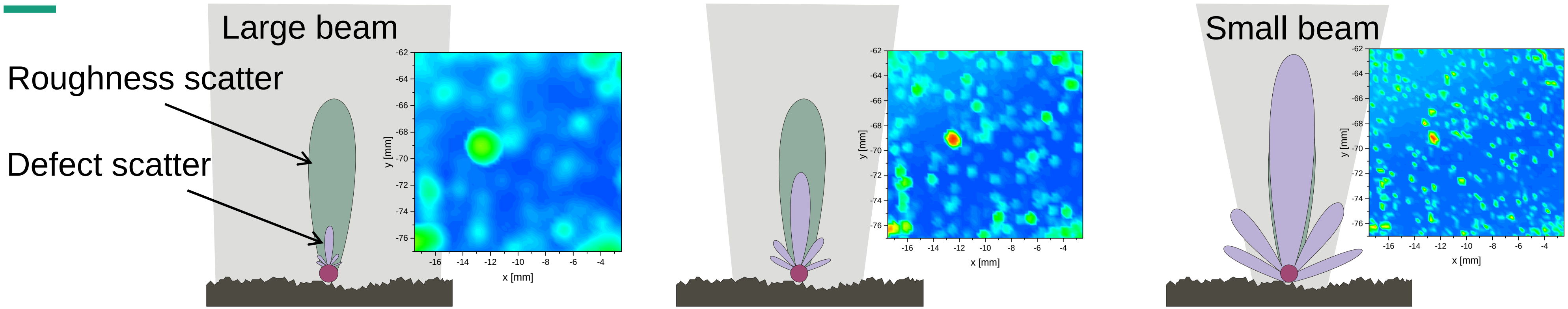
Approaches

Analyzing particle-induced light scattering



Closer to application

Higher resolution / sensitivity

Roughness-induced scatter

- Scatter ~ roughness(²)
- Does not depend on beam diameter

Defect-induced scatter

- Scatter ~ particle size ?
- Does depend on beam diameter

$$ARS(D) = ARS_r(d) + ARS_d(d)\left(\frac{d}{D}\right)^2$$

→ Careful analysis for evaluation of particle induced scattering

→ Averaging to determine **application relevant / area covering** BSDF of contaminated **sample**

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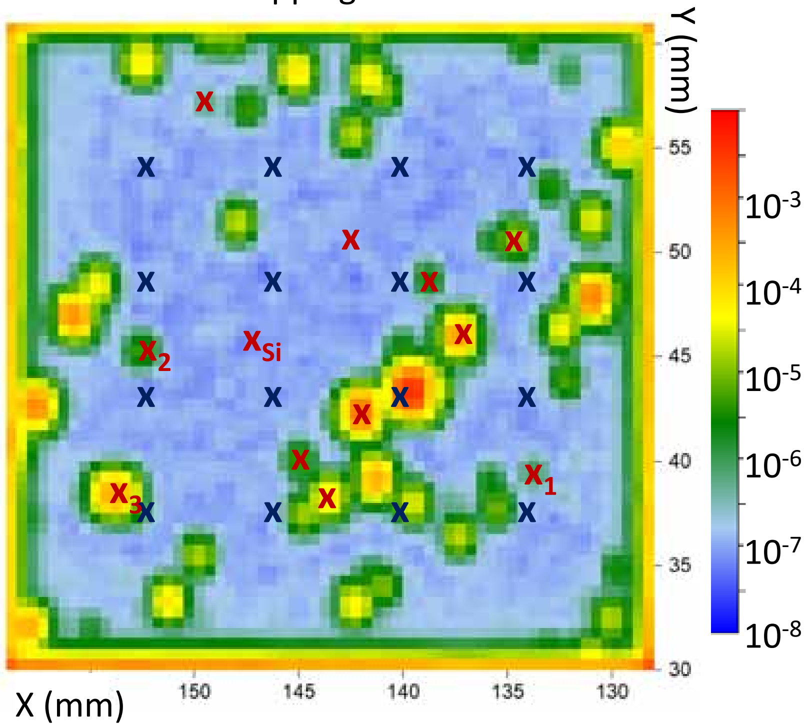
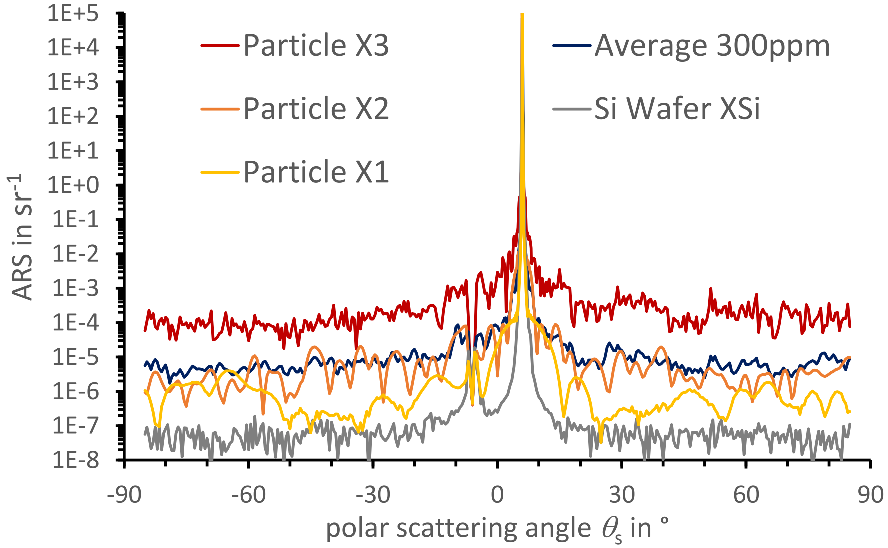
Particle-induced light scattering

Measurement approaches

Silicon mapping at 532 nm





- Particles are localized features
- How to generate a meaningful BRDF of a surface/sample with low stochastic uncertainty and without measuring entire sample?
- Measure all positions? → lasts days

→ **Averaging approaches**

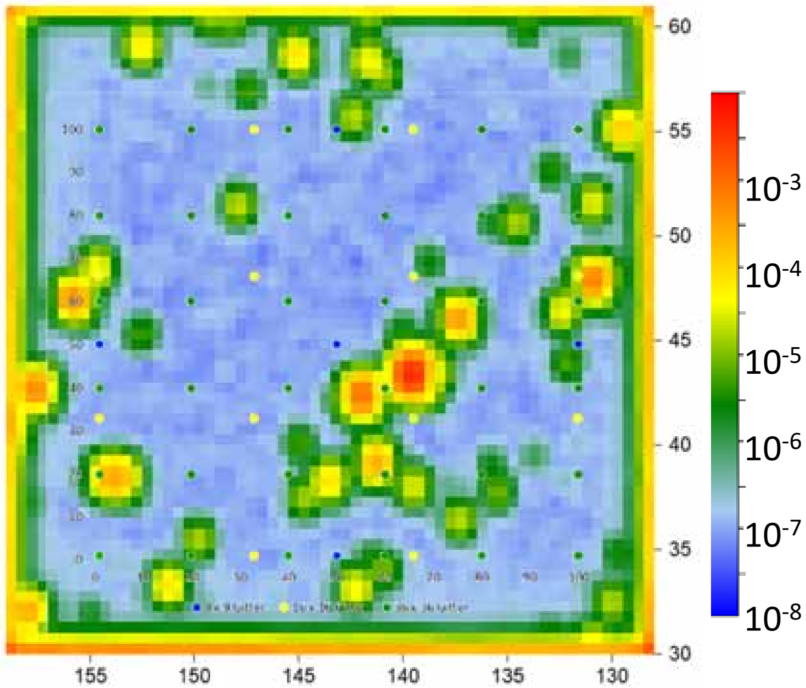
- **OHB approach**: regular pattern
- **IOF approach**: mapping + selected positions

OHB Fraunhofer IOF

Particle-induced light scattering

Measurement approach at OHB

Silicon mapping at 532 nm



OHB approach:

- BRDF measurements for positions on regular pattern → averaging
- Number of measurement positions* according to contamination level and beam size:

Table 1: calculation of needed measurement points

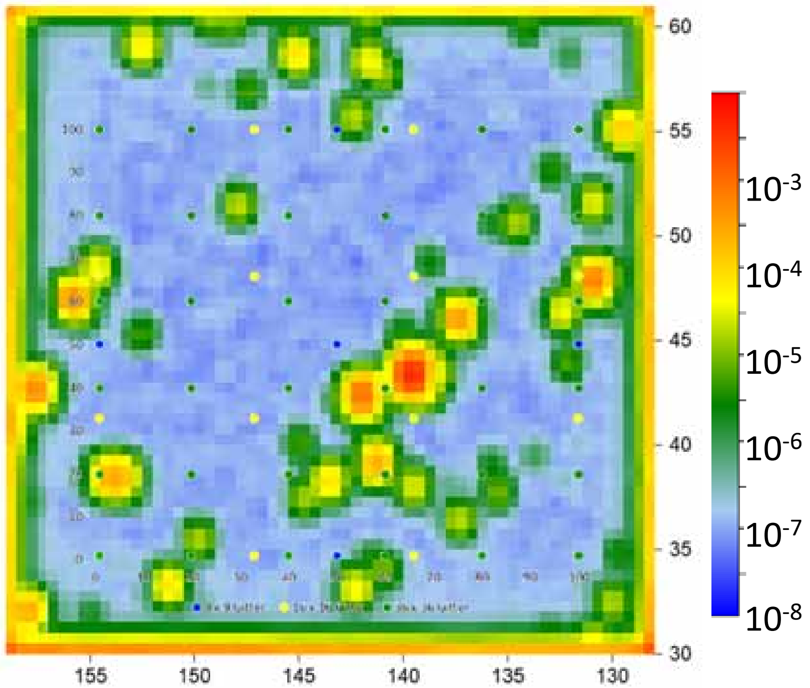
contamination level [ppm]	contamination level [CL]	number of particles in a 3 mm spot		theoretical number of measurement points	used measurement points
20	164.32	2.68		74.76	100
50	204.48	6.69		29.91	36
100	239.85	13.38		14.95	16
300	306.08	40.13		4.98	9
1000	395.31	133.75		1.50	9
5000	547.53	668.76		0.30	9

*discussed and tested in master thesis by A. Althammer who performed BSDF measurements at OHB

Particle-induced light scattering

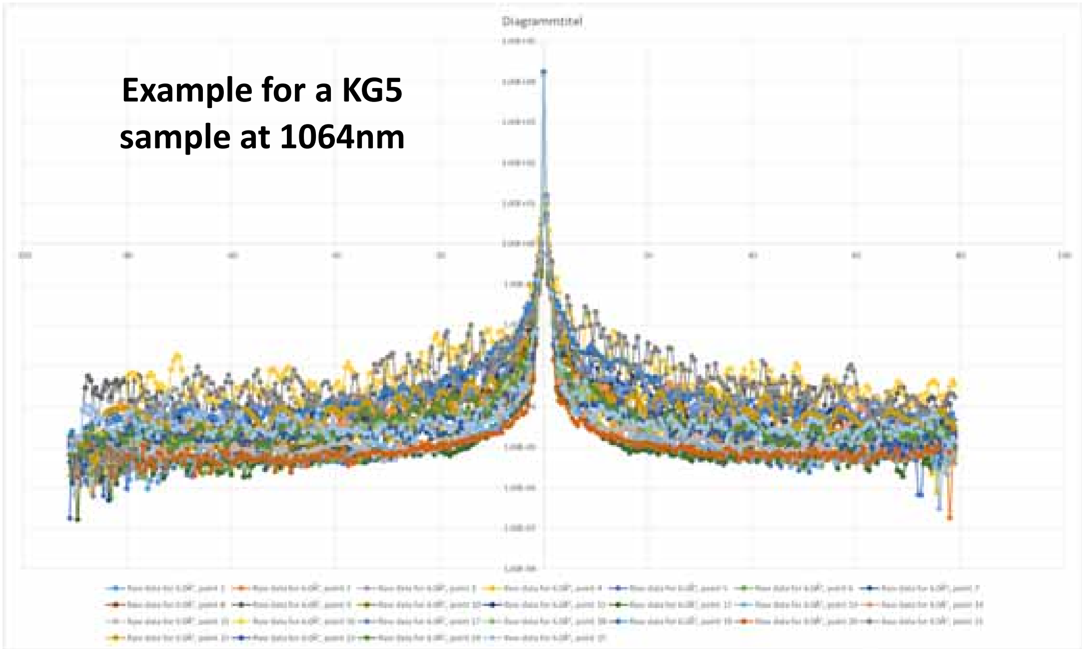
Measurement approach at OHB

Silicon mapping at 532 nm



OHB approach:

- BRDF measurements for positions on regular pattern → averaging
- Scattering results:



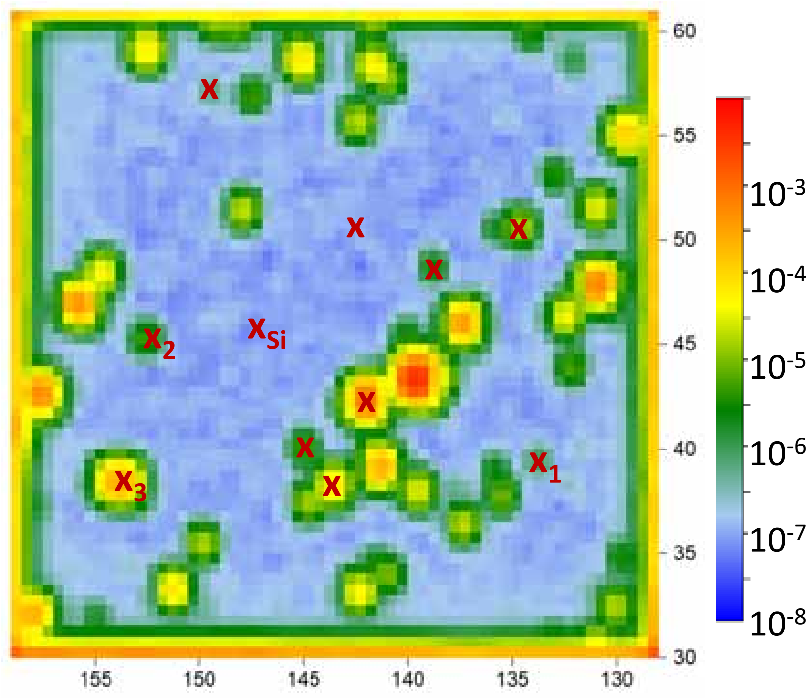
*discussed and tested in master thesis by A. Althammer who performed BSDF measurements at OHB

OHB Fraunhofer IOF

Particle-induced light scattering

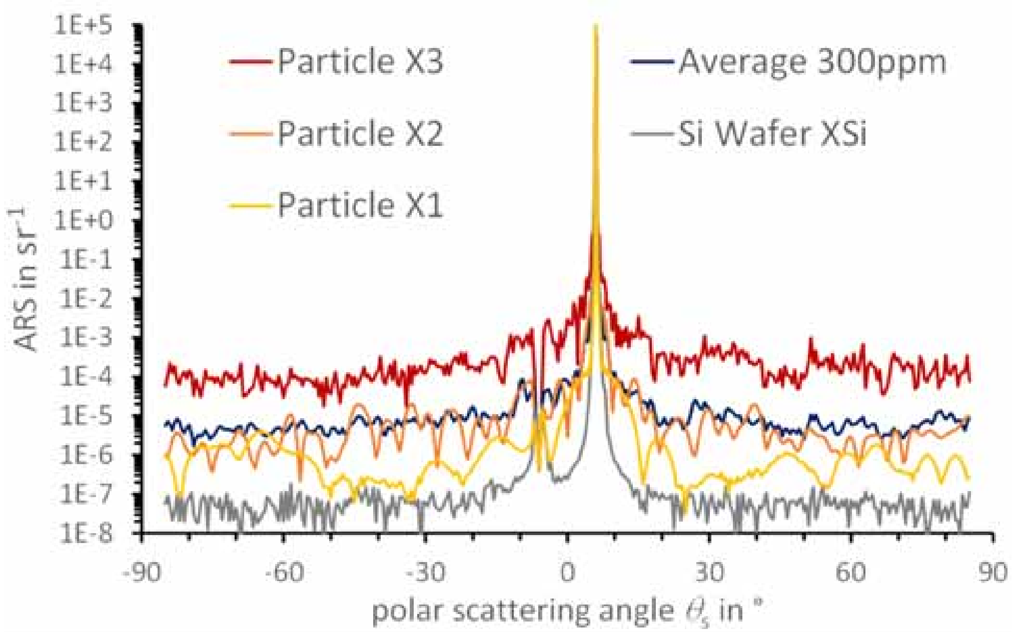
Measurement approach at IOF

Silicon mapping at 532 nm



IOF approach:

- Map the scattering into fixed detection direction for the entire surface
  → Measure BRDF of selected positions & generate histogram
- Average according to histogram



OHB Fraunhofer IOF

Efficient scattering analysis of PAC contaminated samples

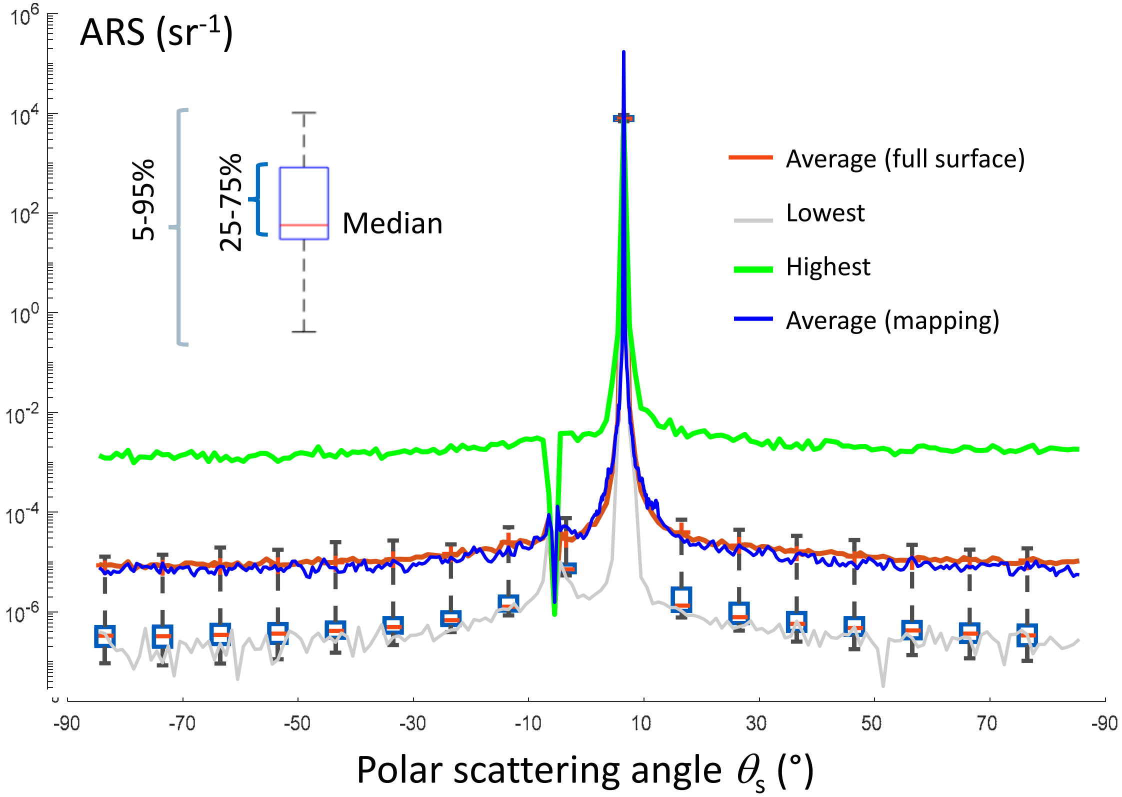
Measurement approach at IOF (cross check)

- Full surface analysis (area:15x20mm² → 70h):

Extended stochastic analysis:

- Clean positions dominate box plot (~75%)
- But: particles dominate average
- **Most dominant scattering from less than 5% of features**

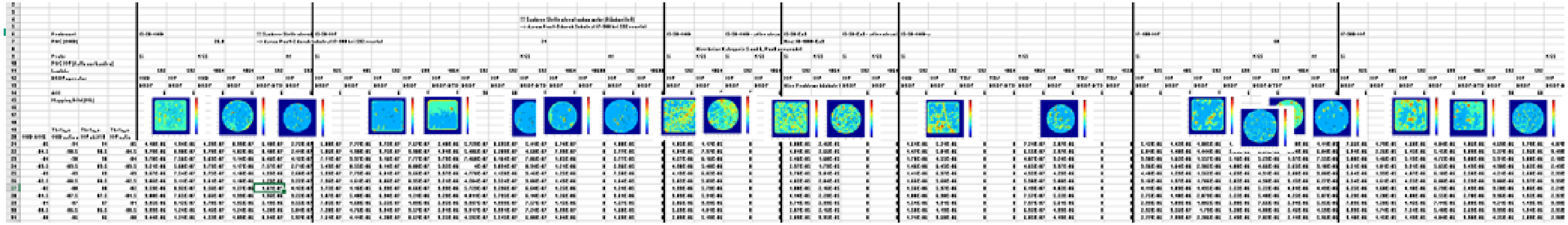
→ Excellent agreement between full surface average and histogram method

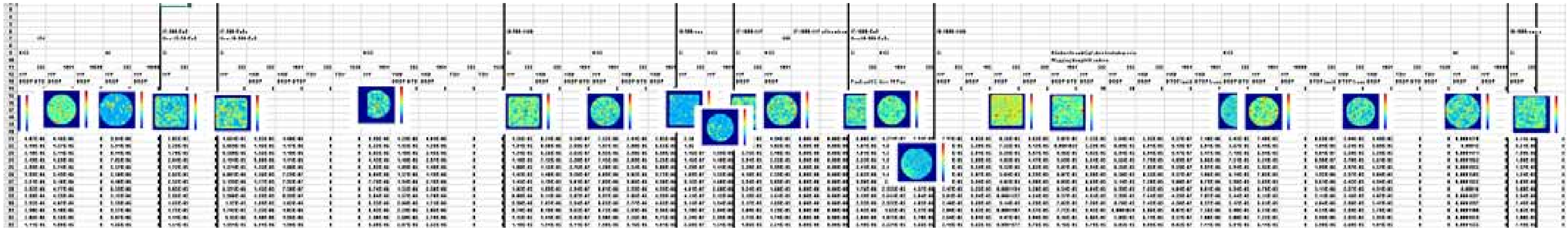


→ Efficient & robust full surface scattering assessment (30x30mm² in 1.5h; +/- 90°)

OHB Fraunhofer IOF

Analysis of all data sets obtained so far





- OHB, IOF and TSW collected 105 averaged curves for the PAC sample sets
- For PAC & MOC ≈ 2000 single BSDF measurements

Agenda / Outline

1. Motivation & Goals
2. Project CoCis
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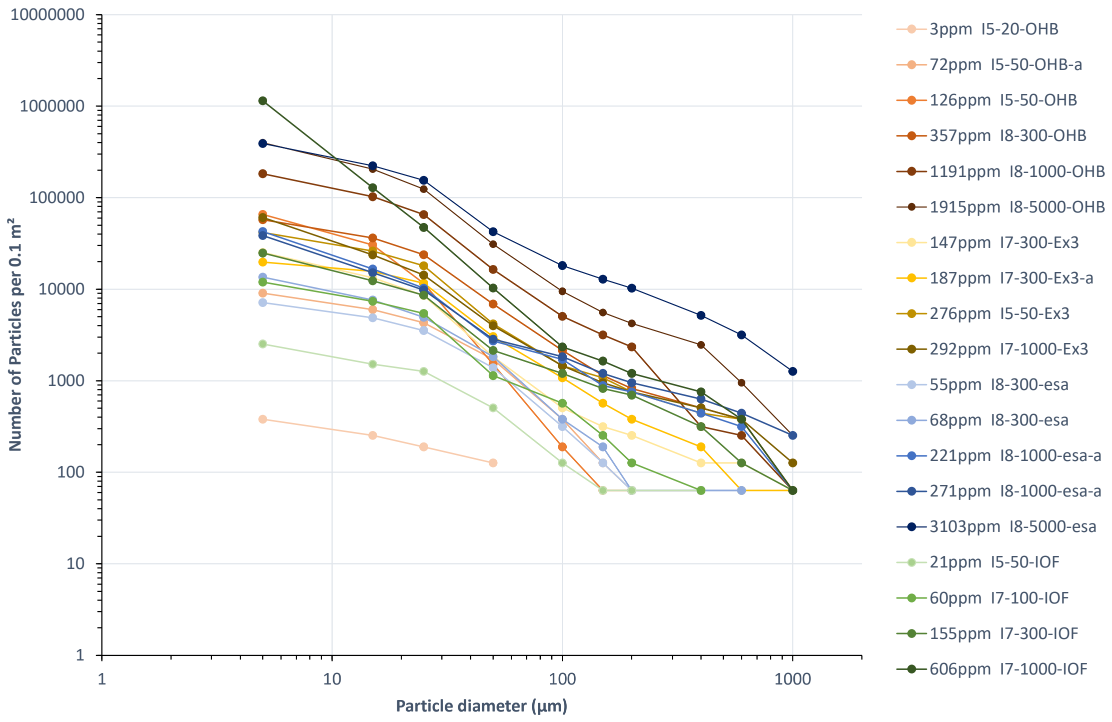
3. Definitions & Approaches
4. Experimental results
   1. PAC fall out results
   2. Scattering from PAC
   3. Scattering from MOC
5. Modelling
   1. Scatter modelling from PAC
   2. Scatter modelling from MOC
   3. Modelling on system Level
6. Summary / Conclusions

Experimental Results - PAC Fall Out

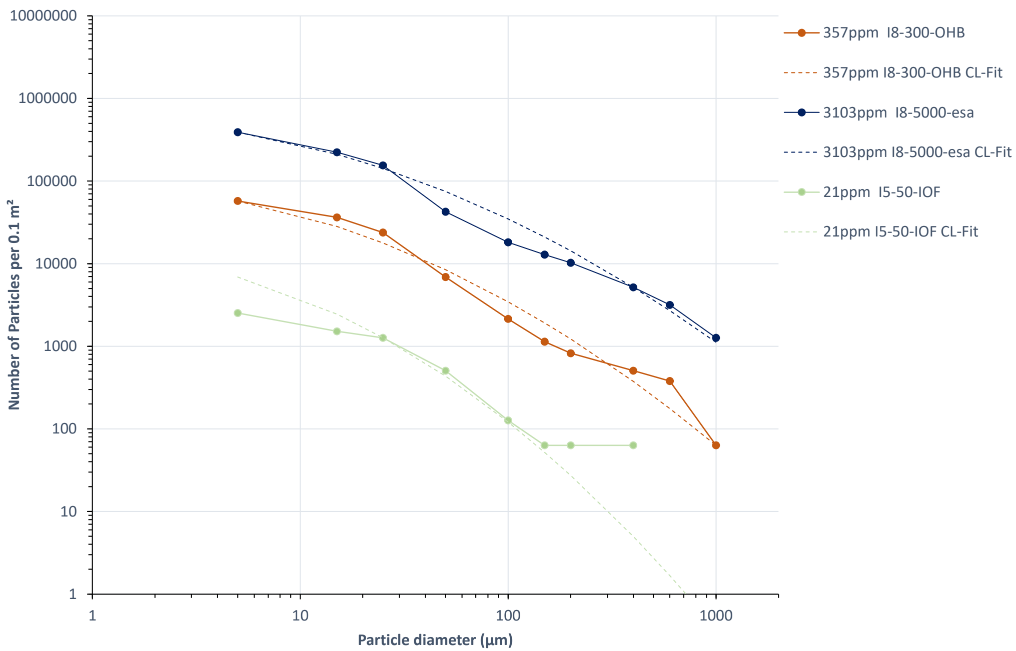
PAC analysis of 17 sample sets

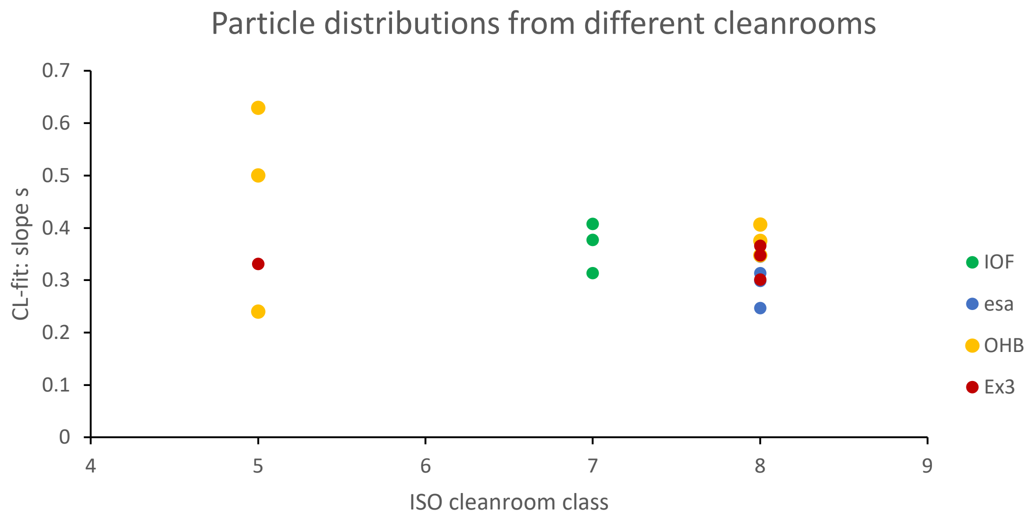
Sample	Clean Room Class	Exposure Time (days)	Achieved PAC in ppm	CL-fit	
				CL	Slope s
I5-50-OHB	I5	186	126	713	0.63
I5-50-OHB-a	I5	72	72	974	0.50
I5-20-OHB	I5	71	3	2376	0.24
I7-300-Ex3	I5	N/A	147	3448	0.37
I7-300-Ex3-a	I8	8	187	3900	0.35
I5-50-Ex3	I8	N/A	276	6301	0.33
I7-1000-Ex3	I8	10	292	9292	0.30
I8-300-OHB	I8	47	357	5829	0.35
I8-300-esa	I8	7	55	2893	0.35
I8-1000-OHB	I8	69	1191	4616	0.41
I5-50-IOF	I5	50	21	720	0.50
I7-100-IOF	I7	19	60	2301	0.38
I7-300-IOF	I7	50	155	6256	0.31
I7-1000-IOF	I7	166	606	4598	0.41
I8-1000-esa-a	I8	14	271	17979	0.25
I8-5000-OHB	I8	302	1915	8392	0.38
I8-5000-esa	I8	397	3103	24118	0.30



- Achieved PAC from 3ppm to 3100 ppm
- CL from 700 to 24000

PAC analysis



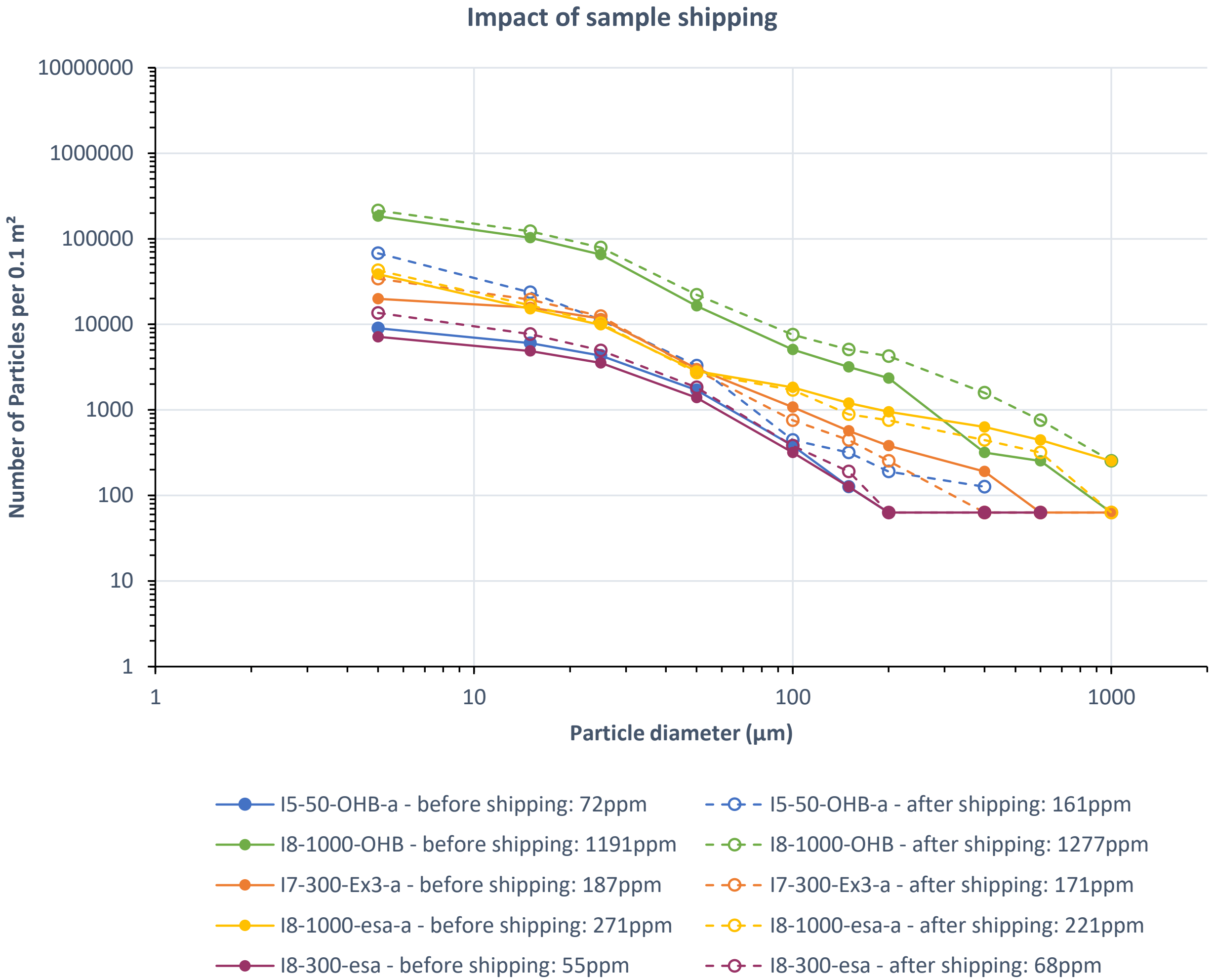


- Reasonable fits of CL & s
- Slope values from s = 0.24 to 0.63

- Higher variety of s for lower clean room classes (lower contamination levels)
- published: s = 0.38 (uncleaned surfaces)

PAC: influence of shipping

- moderate changes in the PAC distribution/level (≲ 10%)
- Slight but no systematic change of PAC slope
- One exception:
  increase of factor 2 for one sample from initially 72ppm to 161 ppm



PAC influence of cleaning

- 4 sample sets, 2 cleaning approaches:

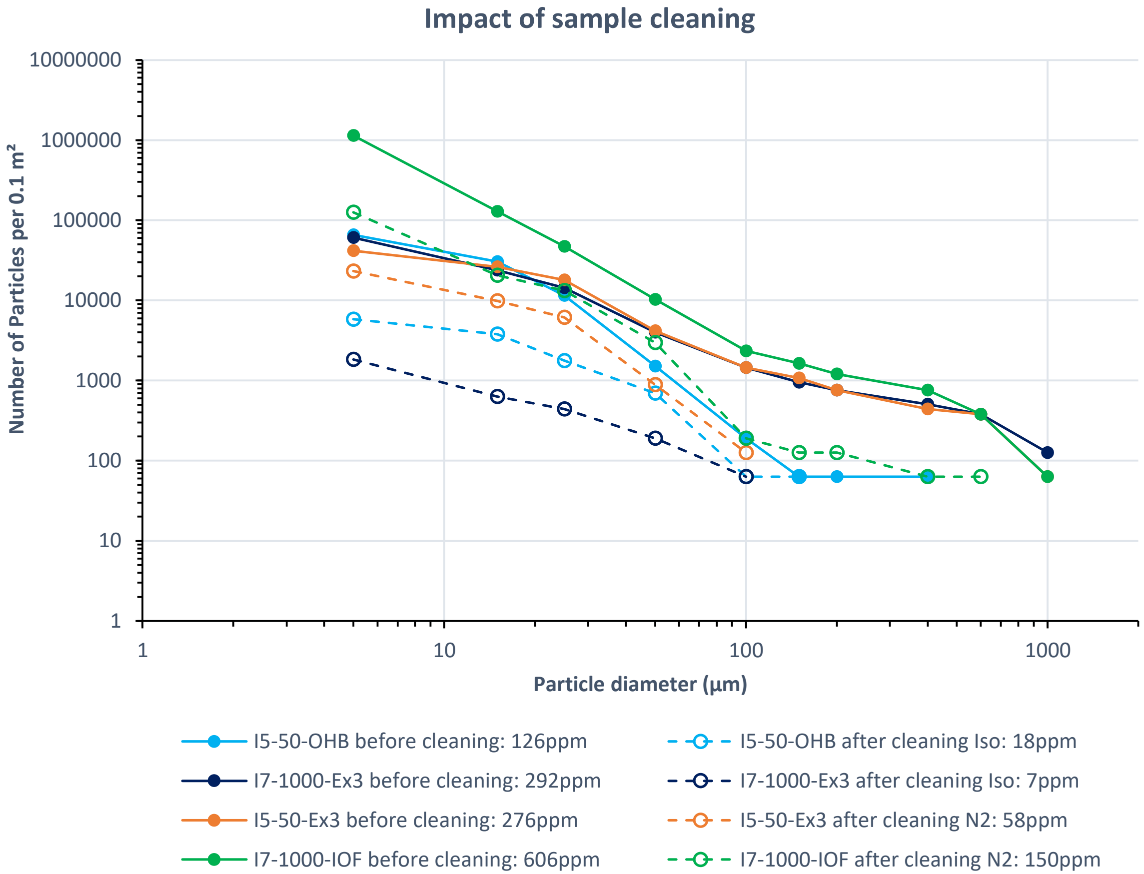
→ **N2 purge**
(sample sets I5-50-Ex3, I7-1000-IOF)

→ Wiping using clean room **microfiber cloth** soaked with **isopropanol**
(sample sets I5-50-OHB, I7-1000-Ex3)

- Significant PAC reduction in particular big particles
- Slope parameter:
s = 0.4 … 0.7 (Literature: 0.9)

- Higher efficiency for wiping

→ Interesting light scattering results



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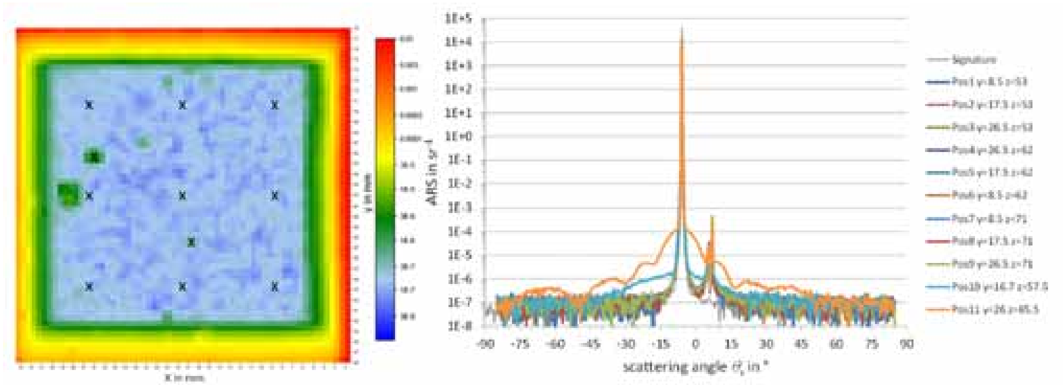
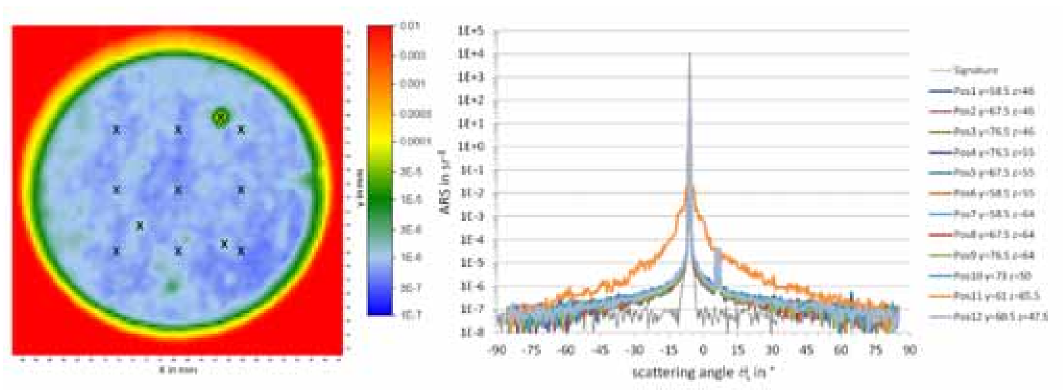
Experimental Results - PAC scattering

OHB Fraunhofer IOF

Initial Scattering Screening





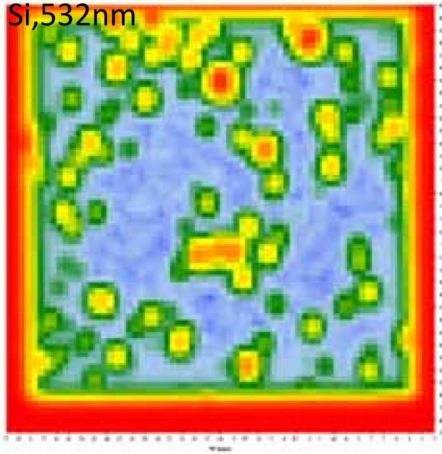
- Prescreening of selected samples regarding PAC and roughness

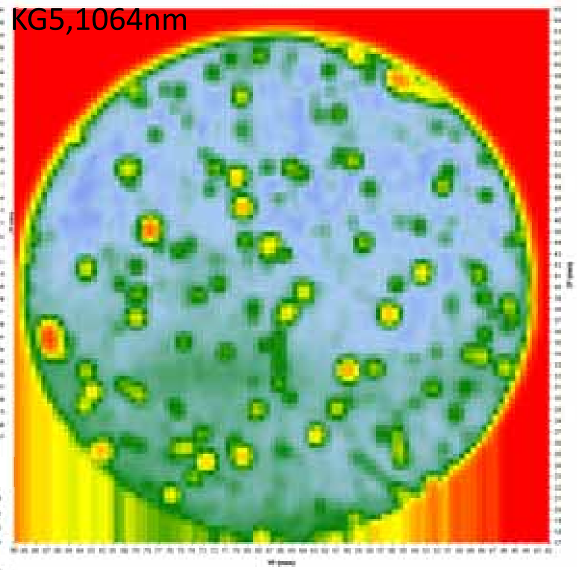
→ High homogeneity, cleanliness and low roughness/initial scattering demonstrated

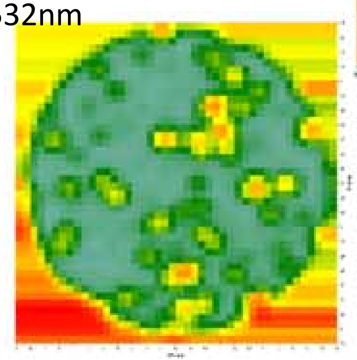
- Only single particles and defects observed

Scattering Mappings

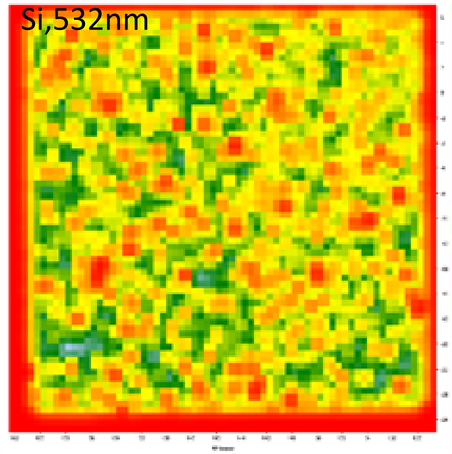
I7-300-IOF, 155ppm

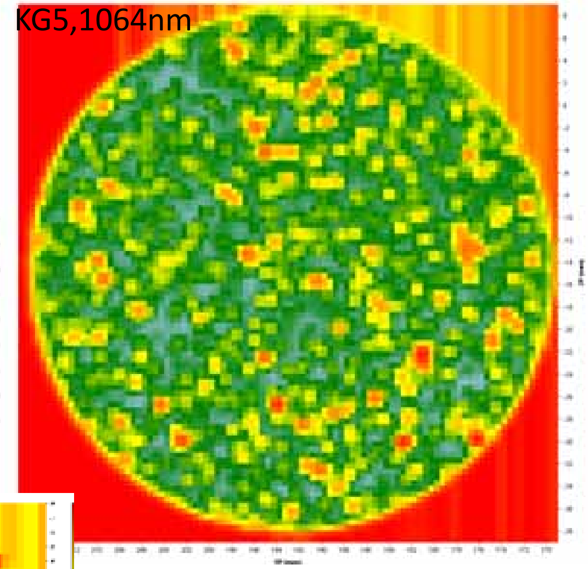


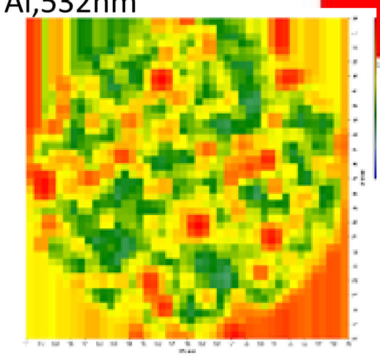




I8-1000-OHB, 1190 ppm



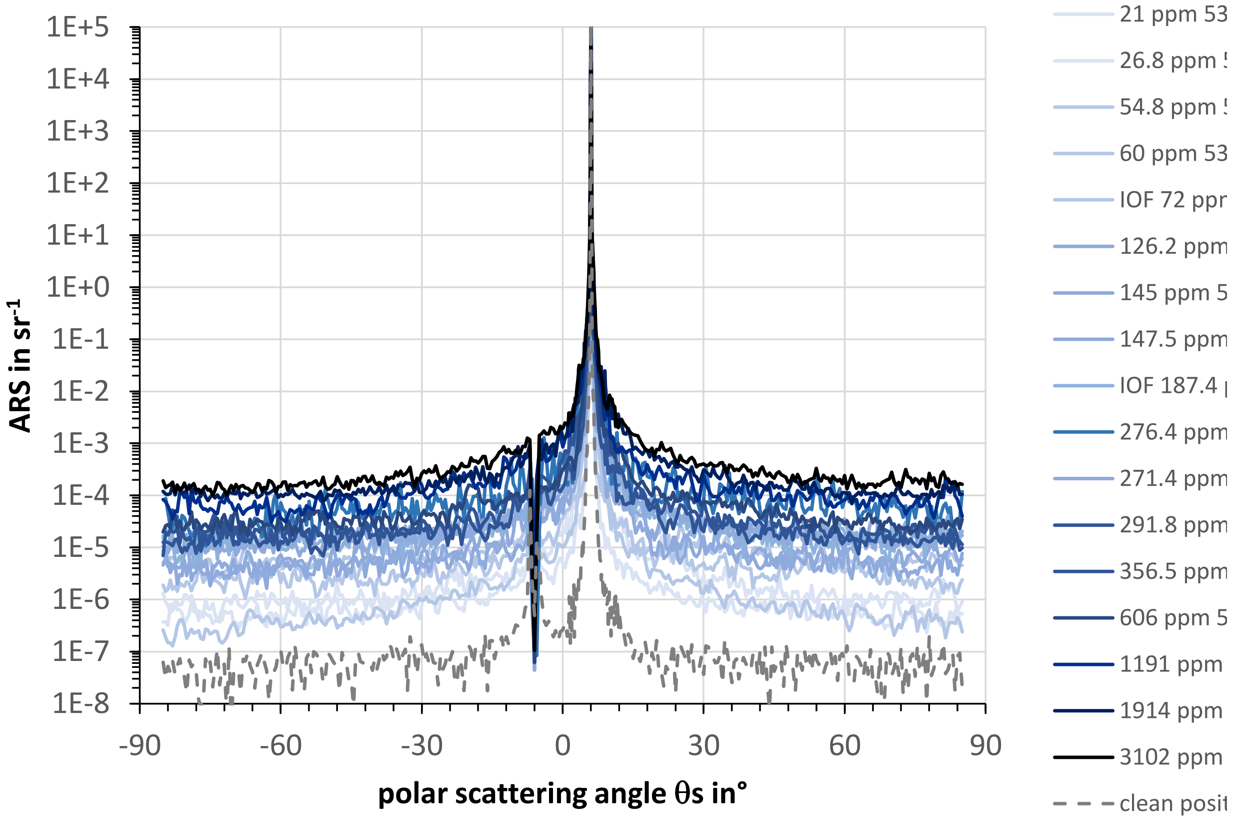




→ Higher PAC primarily causes higher feature density

Scattering of PAC contaminated samples

Silicon at 532 nm

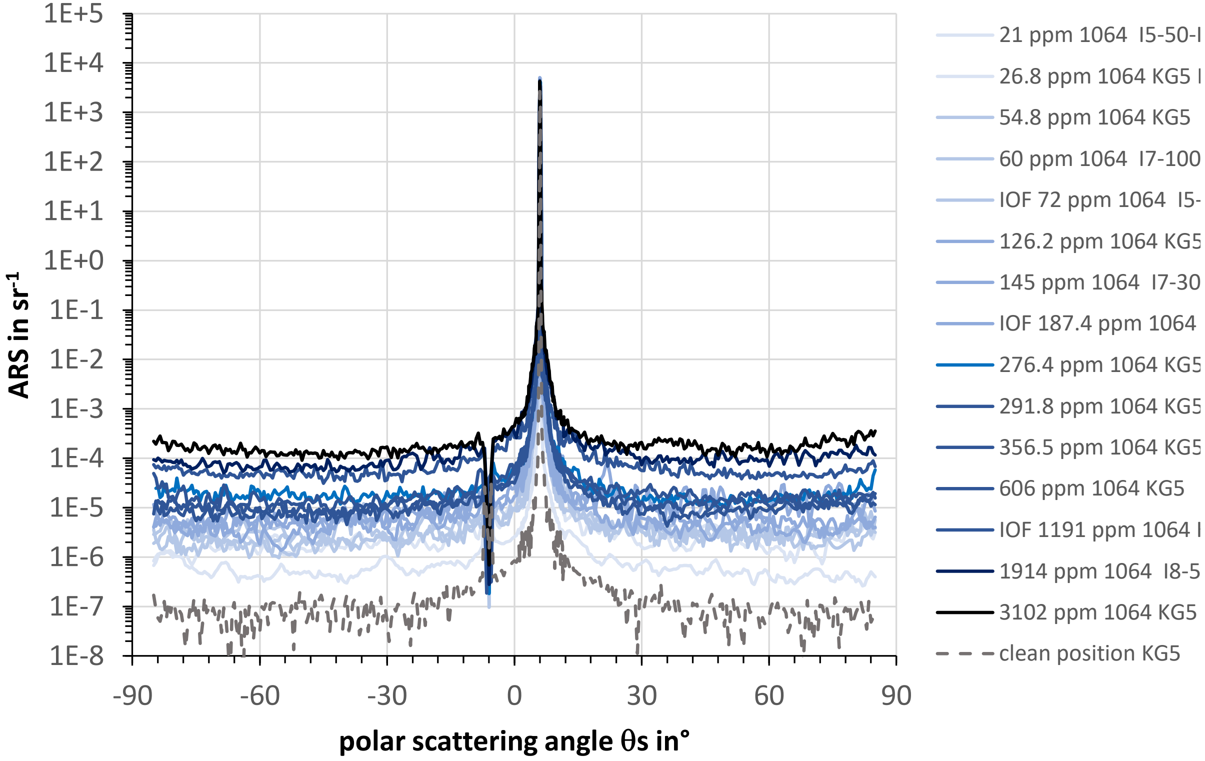


- Percent Area Coverage (PAC): 20 ppm to 3100 ppm
- PAC & size distribution by microscopy, required for later modelling
- **Scattering: increase by >10^3**
- **≈ Linear scaling with PAC ?**

OHB Fraunhofer IOF

Scattering of PAC contaminated samples

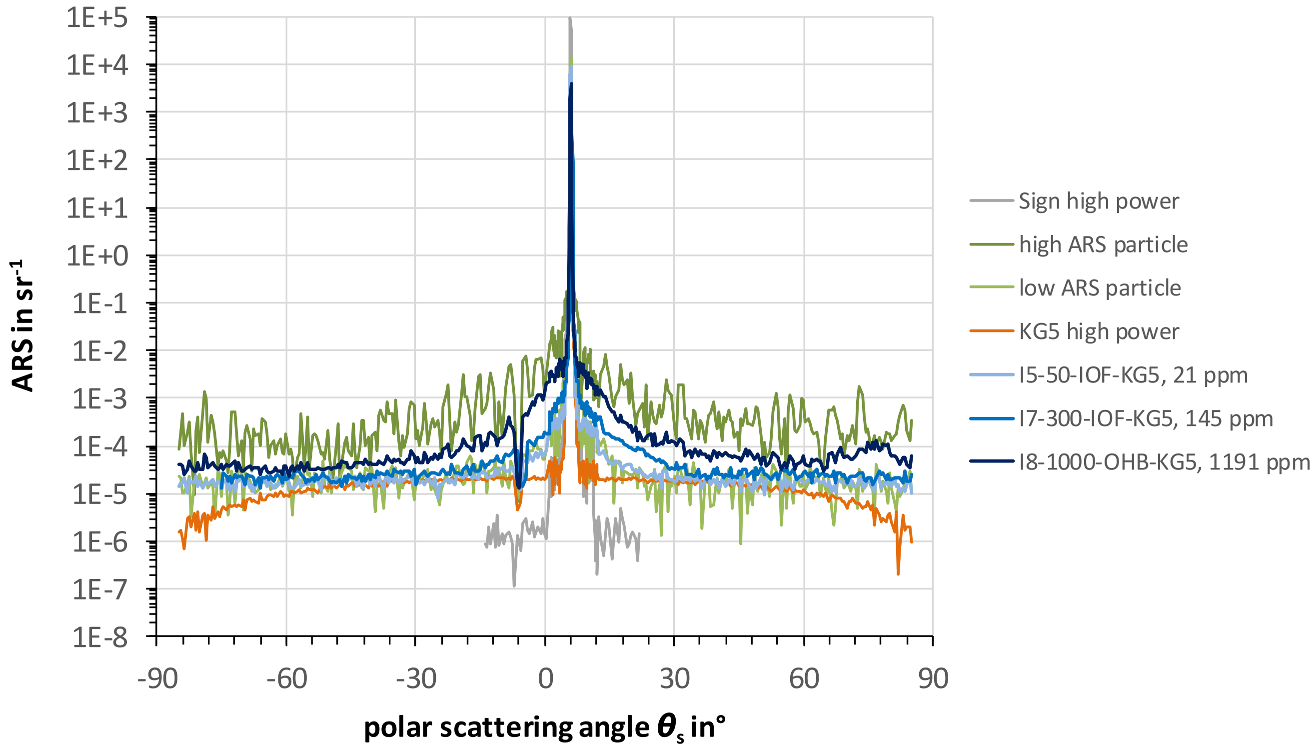
KG5 at 1064 nm



- Percent Area Coverage (PAC): 20 ppm to 3100 ppm
- PAC & size distribution by microscopy, required for later modelling
- **Scattering: increase by >10^3**
- **≈ Linear scaling with PAC ?**
- Slightly different high angle slope than for PAC on Si at 532nm

Scattering of PAC contaminated samples

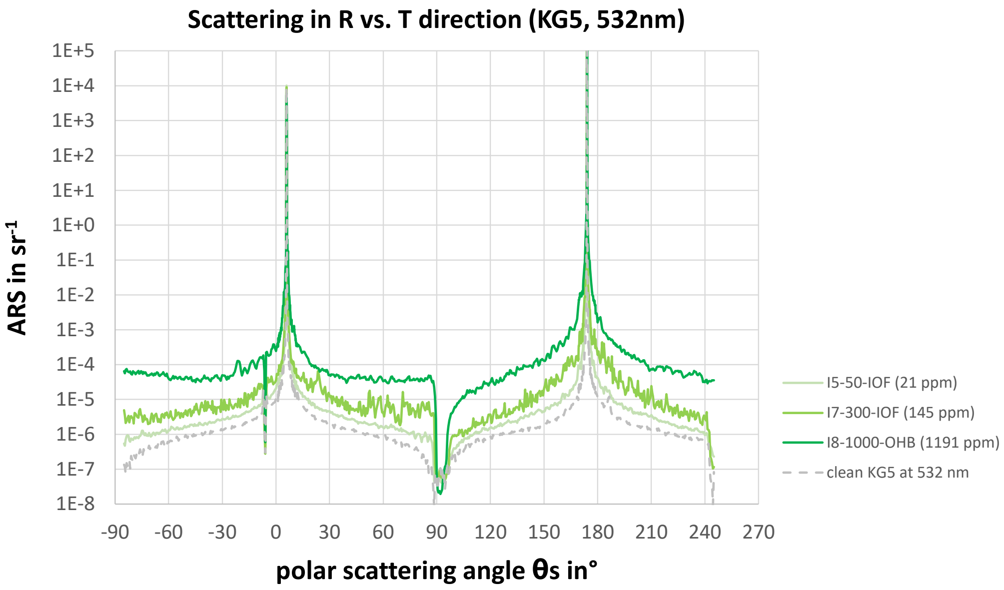
KG5 at 10600 nm

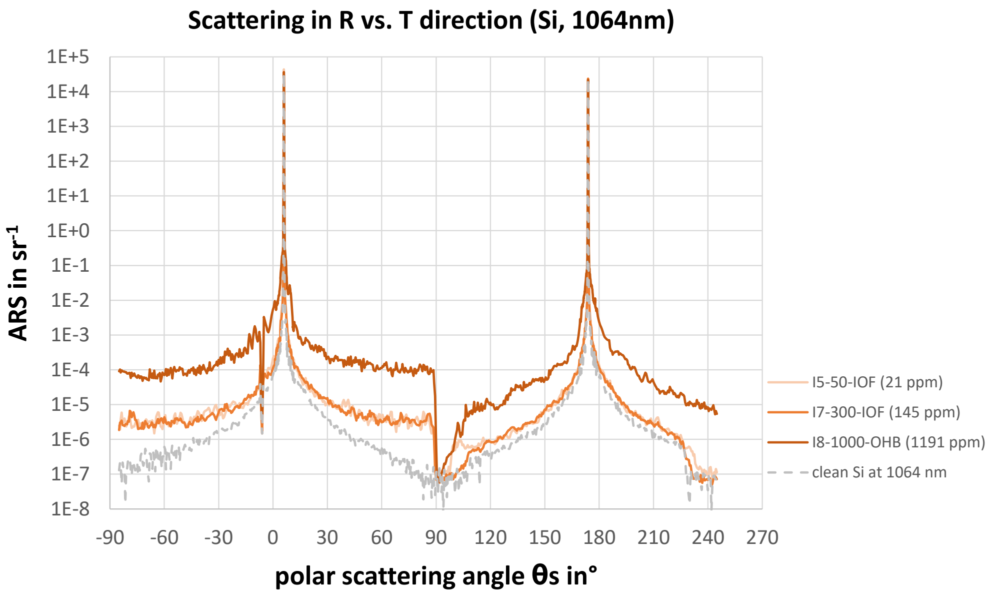


- 3 KG5 samples also analyzed at 10600 nm
- In general measurements and quite similar behavior as for VIS wavelengths
- However, thermal effects of glass or instrument noise becomes critical

Scattering of PAC contaminated samples

transparent sample





- Influence of backside scattering → increase of scattering for clean sample
- Different slope for scattering transmission → BTDF closer to substrate induced scattering

→ Please see modelling results

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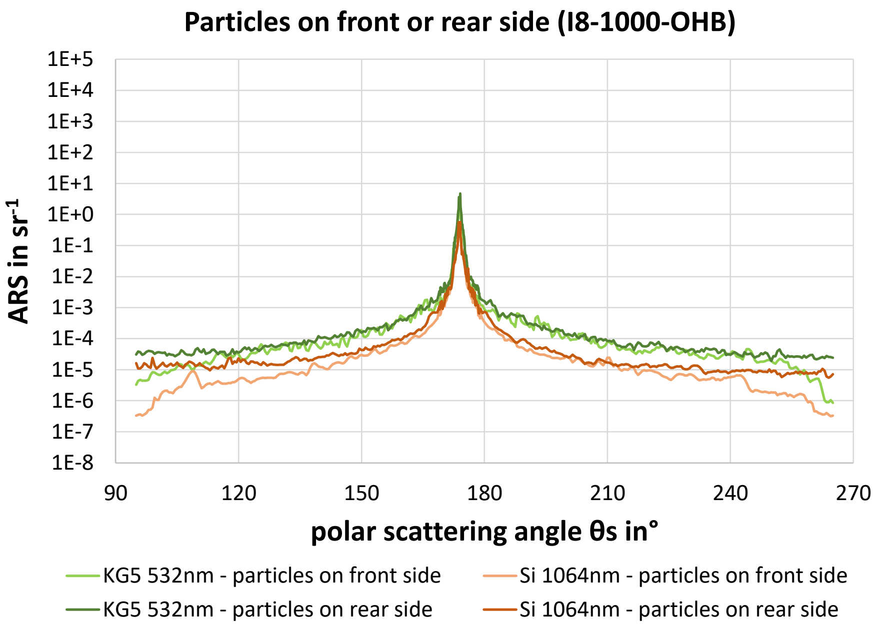
Scattering of PAC contaminated samples

Particles on front or rear side

Forward scattering,



- Test at OHB: Forward scattering with particles on front vs. rear side
- Slight difference for KG5 (at 532nm)
- Higher differences for Si (at 1064nm)
- Increasing differences at higher scattering angles

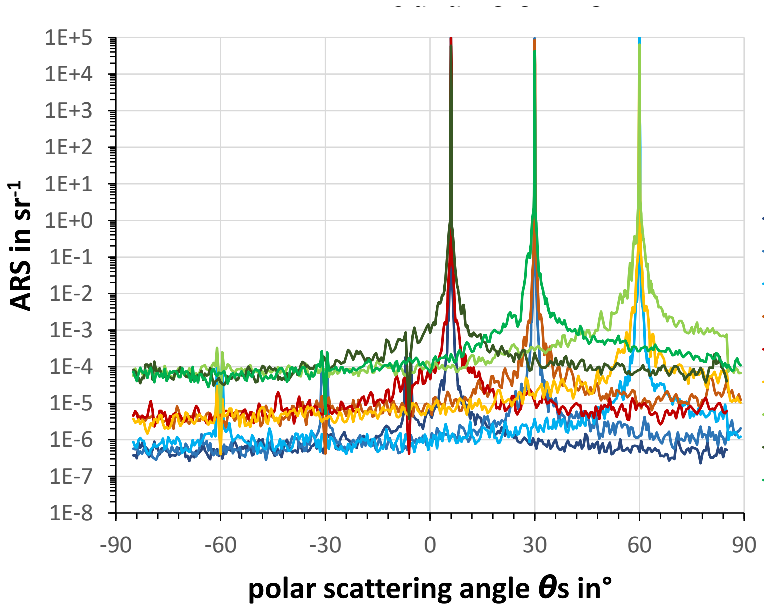
→ Higher scattering for particles on exit surface

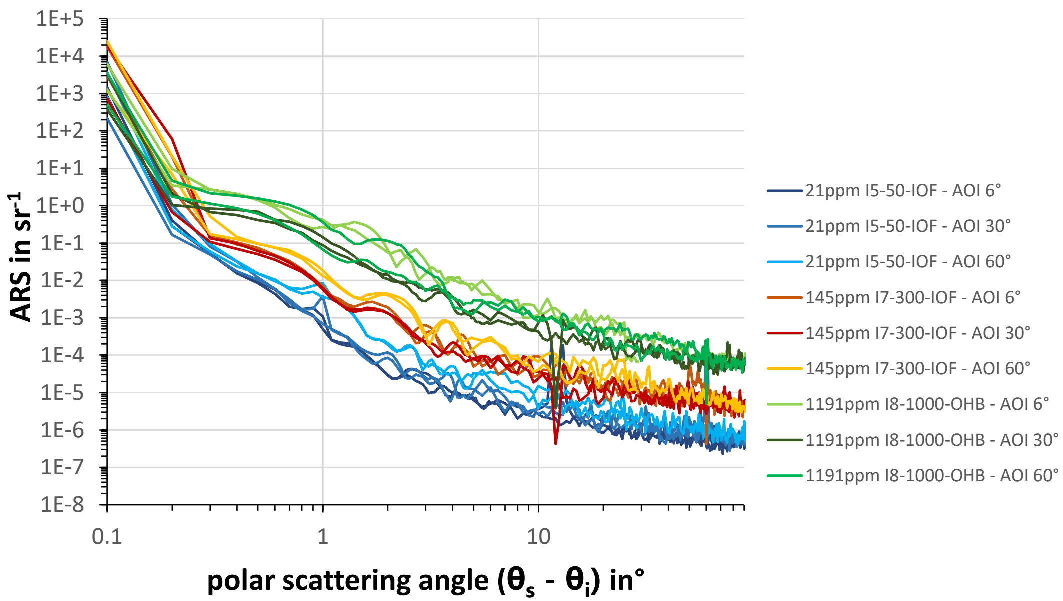
→ Caused by: reflectance / transmission / absorption + geometric effects

→ See Modelling for further explanation

Scattering of PAC contaminated samples

Influence of incidence angles

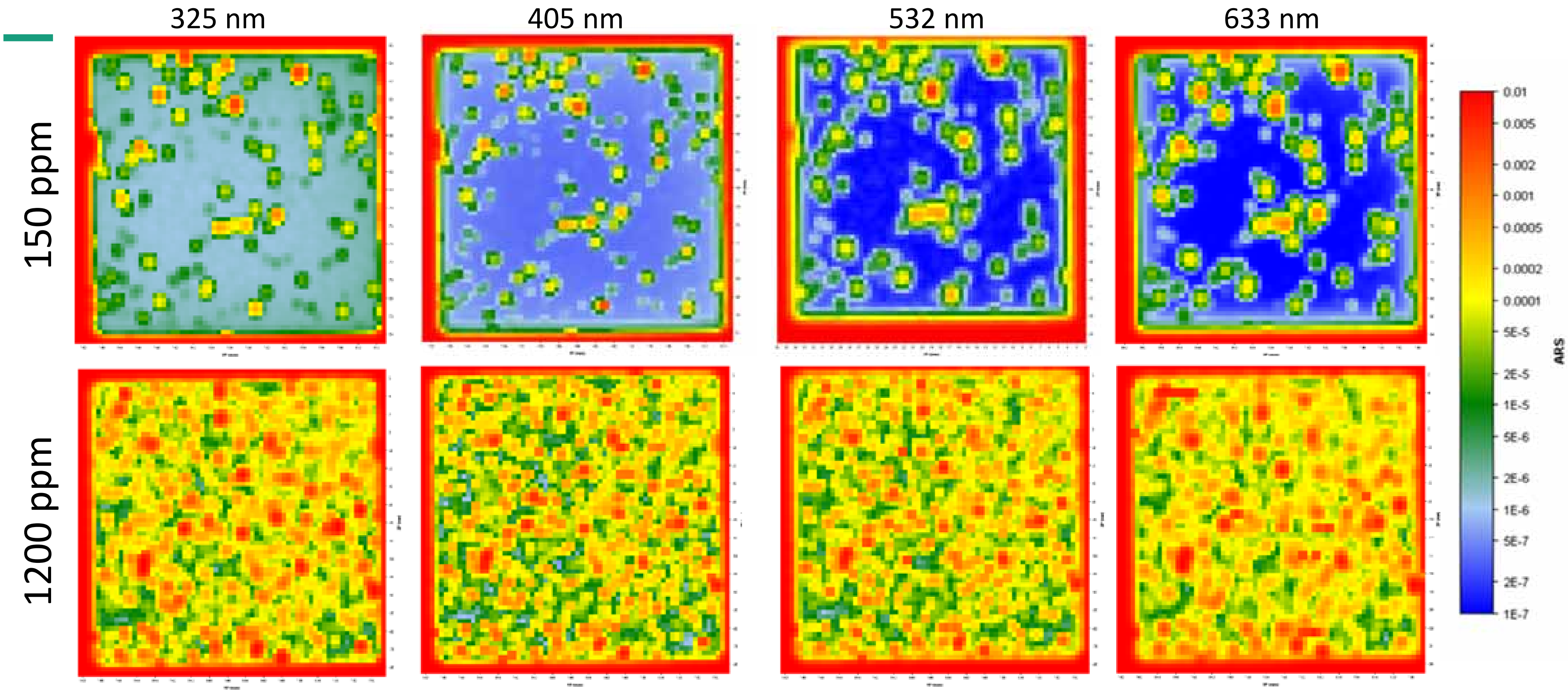




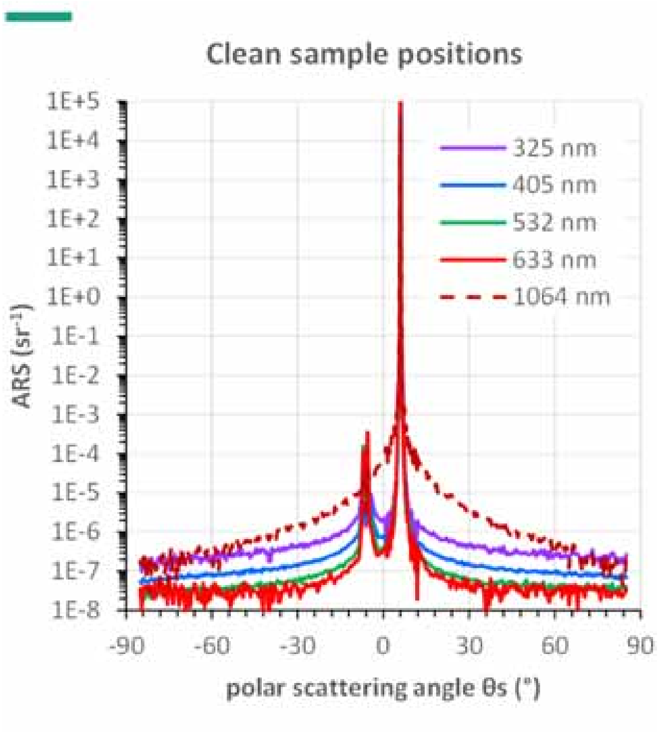
- Oscillation behavior not much changing
- Only moderate changes in level, in particular close to specular direction

→ Particle forward scattering scaled by changing reflectance of the surface?

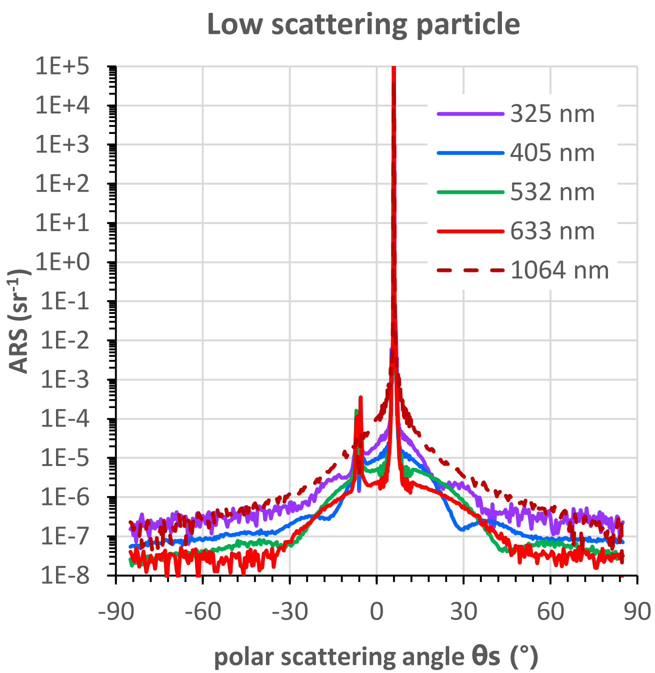
Wavelength and PAC scaling (Silicon wafer)



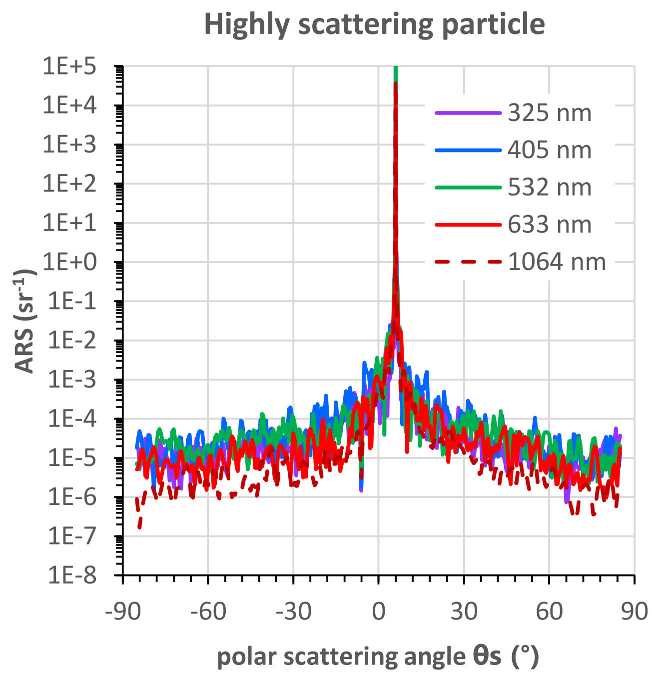
Scaling of SINGLE particle induced scattering



- Roughness induced scattering $\propto 1/\lambda^4$



- Small particles $\propto 1/\lambda^4 \ldots \lambda^2$
- Diffraction acc. to λ

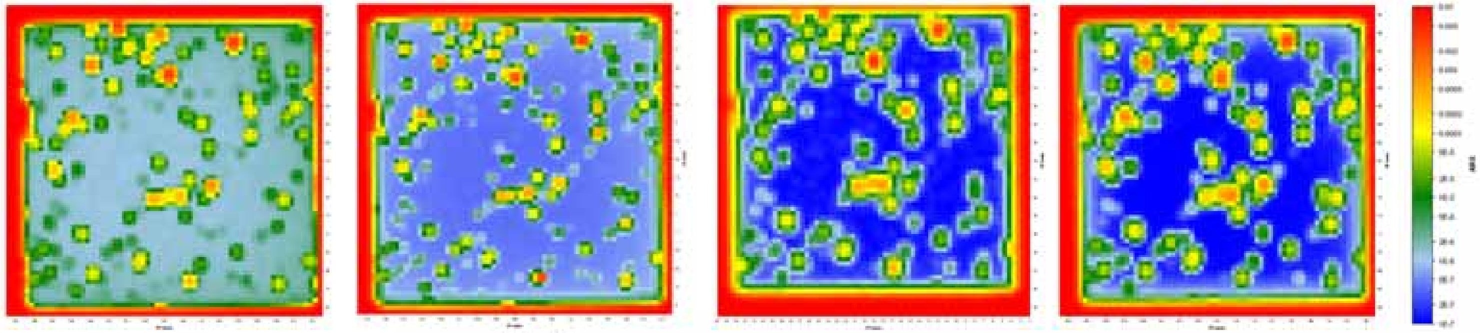


- λ ??
- High oscillation density ("speckle")

Experimental results: scaling of particle induced scattering

Wavelength scaling
Si sample, 300 ppm

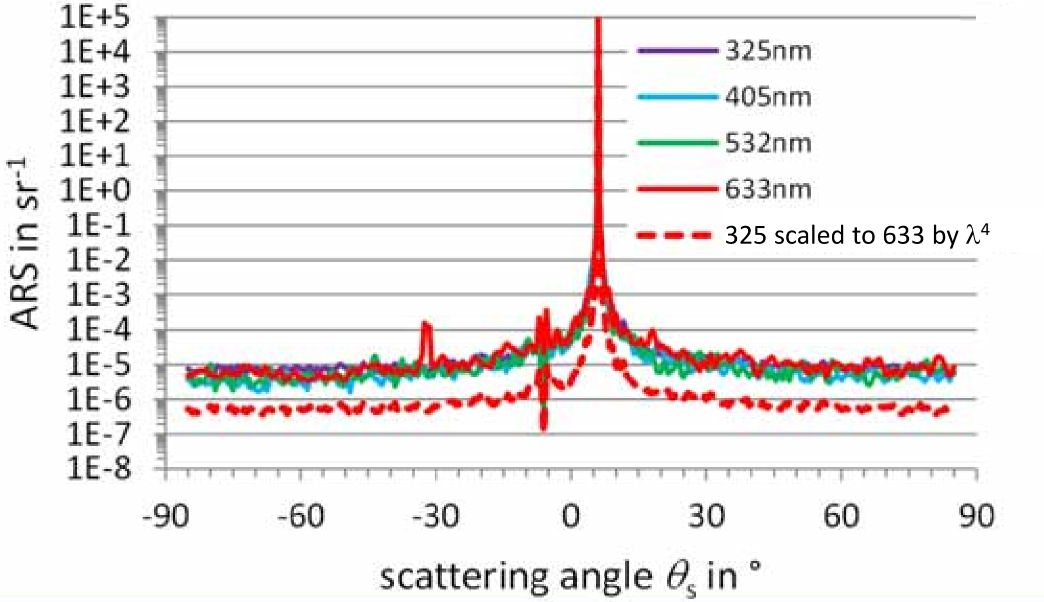
325 nm | 405 nm | 532 nm | 633 nm



- Particle free regions:
  scaling according to ≈1 /λ^4
  (roughness induced Rayleigh scattering)

- Averaged curve of contaminated sample:

  No significant wavelength scaling (scattering dominated by particles >> λ)



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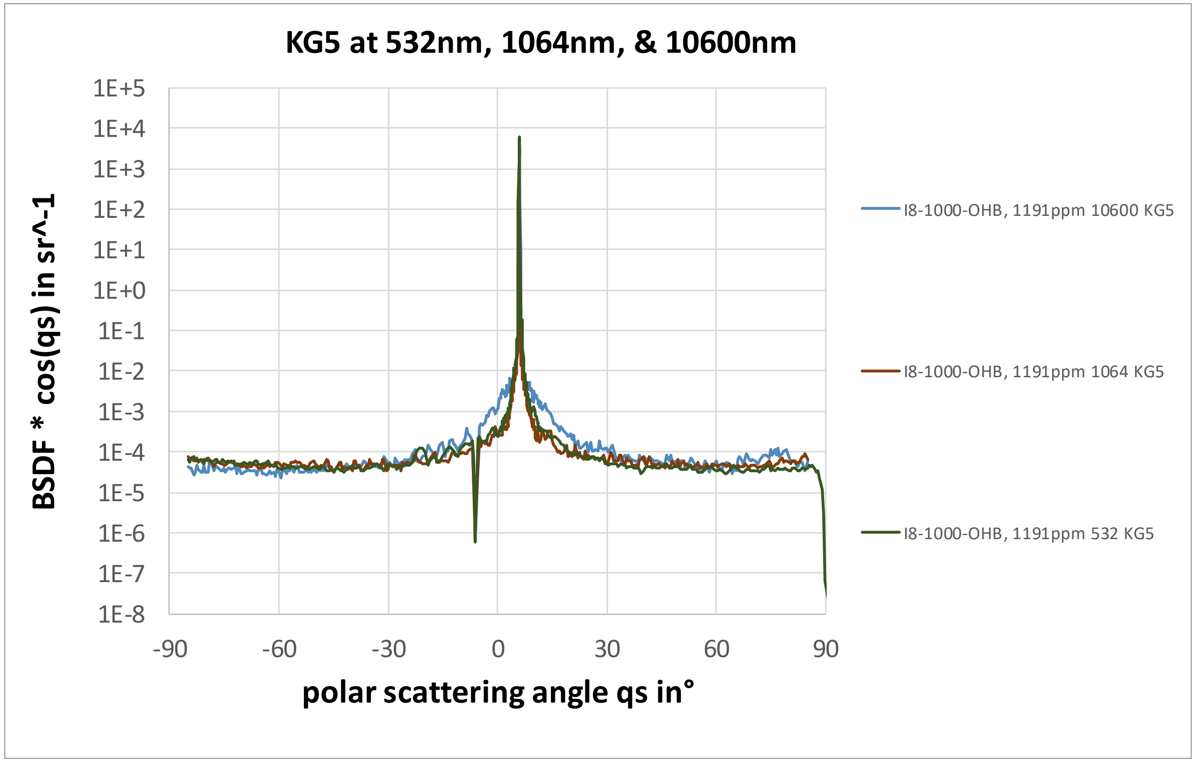
Experimental results: scaling of particle induced scattering

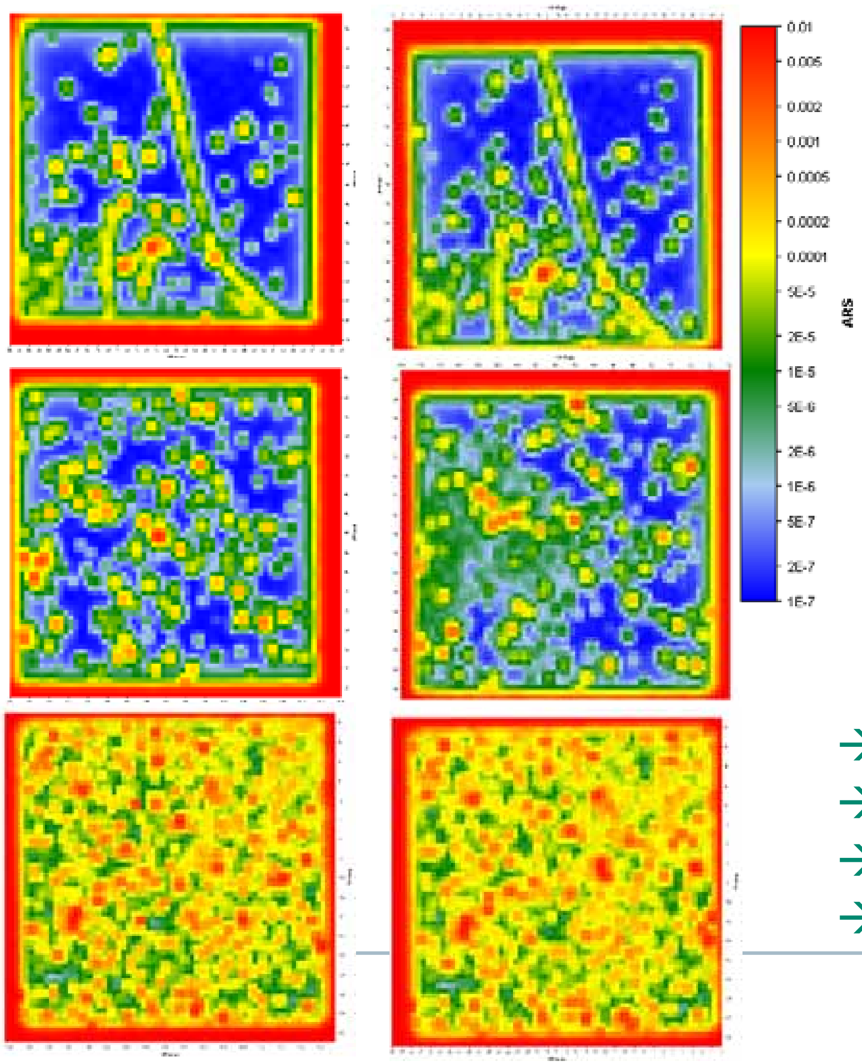
Wider wavelength range

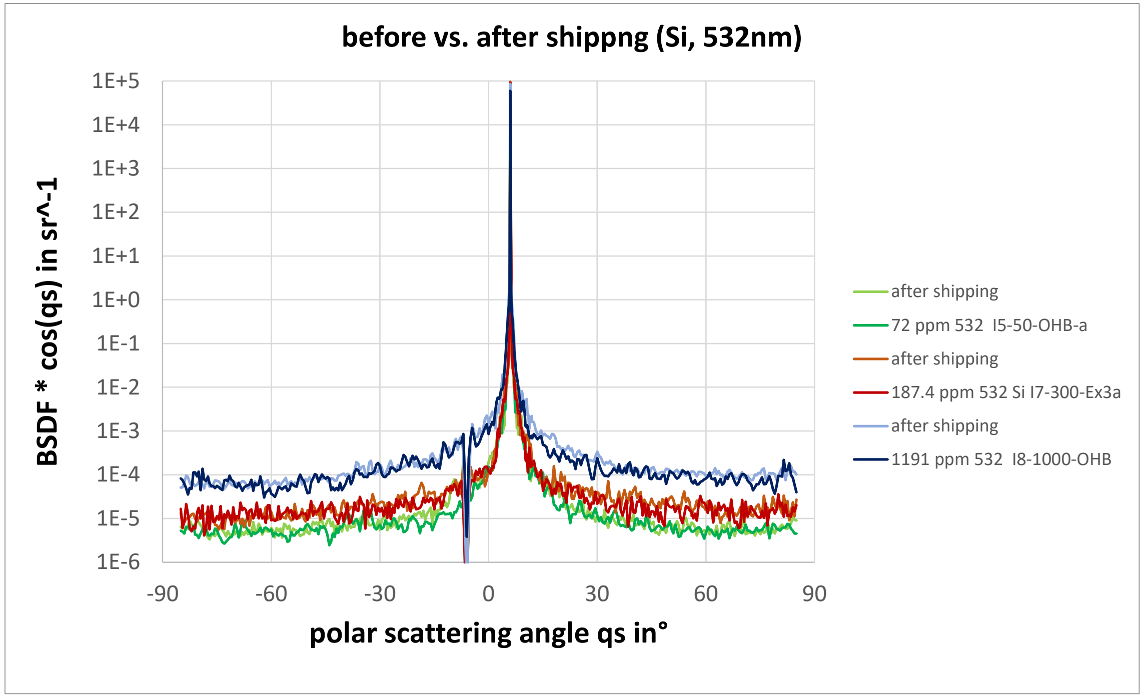


- No significant wavelength scaling at higher scattering angles
- Changes in +/-20° to specular direction

→ Effect of particle becoming appr. or smaller than the wavelength (see modelling)

Scattering of PAC contaminated samples - Before vs. after shipping (Si, 532nm)





- → Most features stay identical / similar
- → Alterations for sample with medium contamination level
- → Almost no changes for averaged curves
- → (same for KG5 at 1064 nm)

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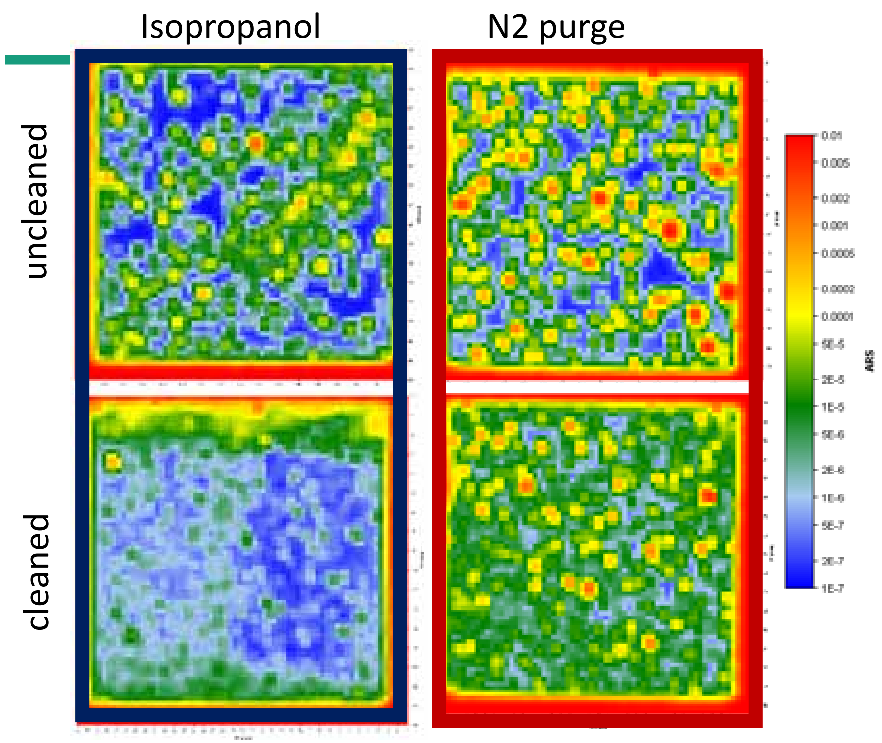
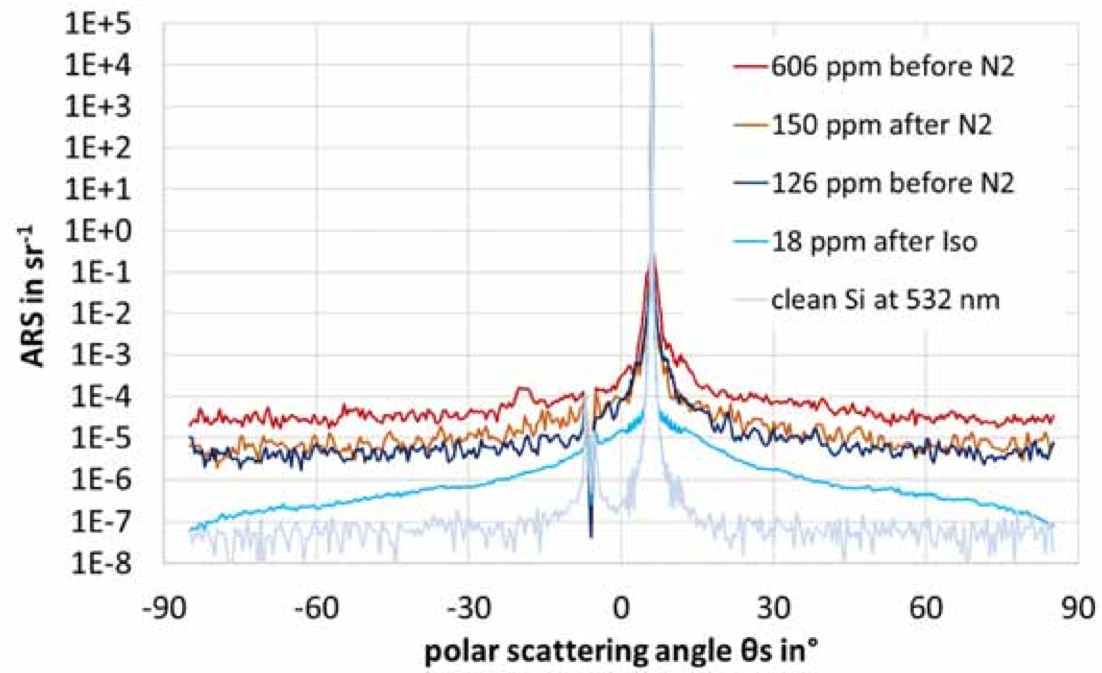
Analysis before and after cleaning - Isopropanol wiping vs N2 purge





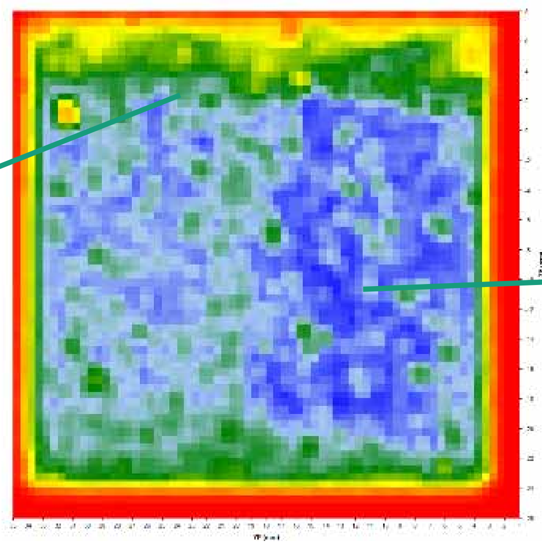
- Significant reduction of averaged scattering level, but "redistribution" in particular for N2
- Isopropanol: Big and medium sized particles removed, but "haze" induced
  → **dominant scattering by particles ~1-2µm (see modelling)**

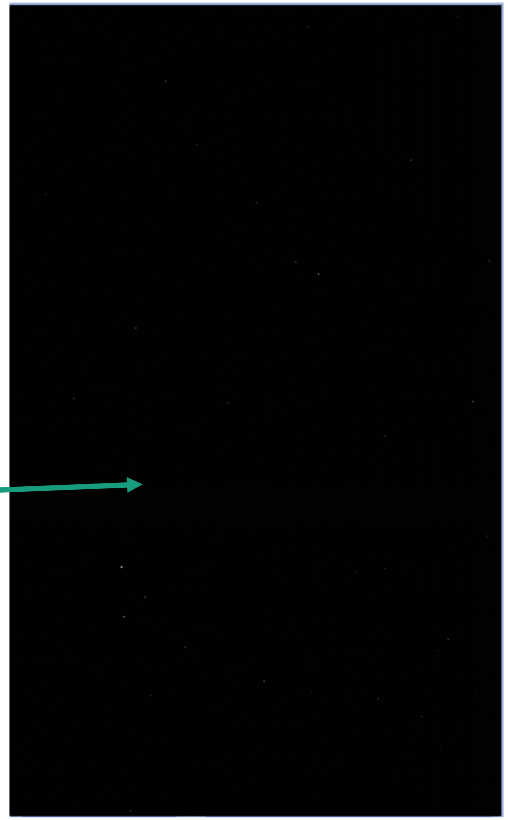
OHB Fraunhofer IOF

Analysis before and after cleaning

Isopropanol wiping

- High variation in small particle density for solvent cleaning
- Particles with diameters of 1 to 4 µm





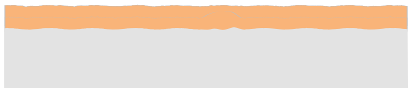
Agenda / Outline

Experimental Results - MOC scattering

MOC – Molecular Organic Contamination

- MOC: source of absorption & “spectral disturbance”
- MOC formation ??

→ Application of particle model(s) ?

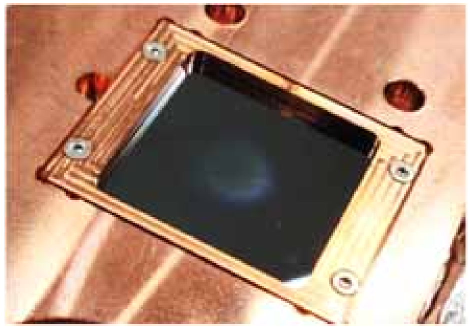


Thin film MOC (nm range)

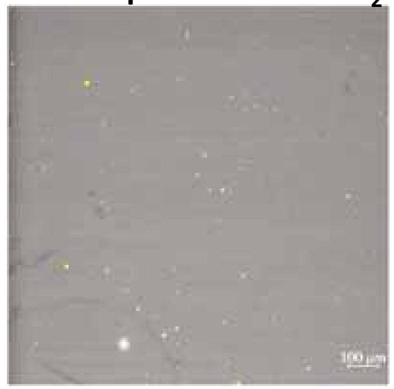
→ Application of thin film roughness scattering models ?

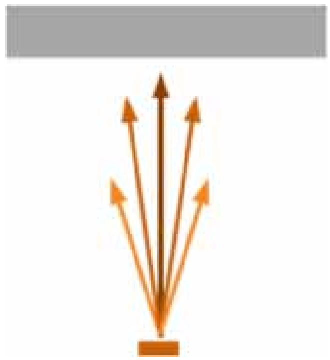
- MOC contamination @ esa-ESTEC (Effusion cell)
- Contaminants: Epoxy **EC2216**, Silicone Elastosil RT745

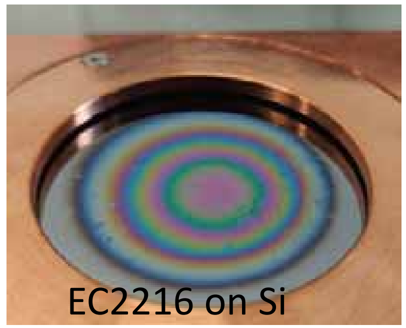
EC2216 Haze on Si



acr. adhesive “particles” on CaF_2



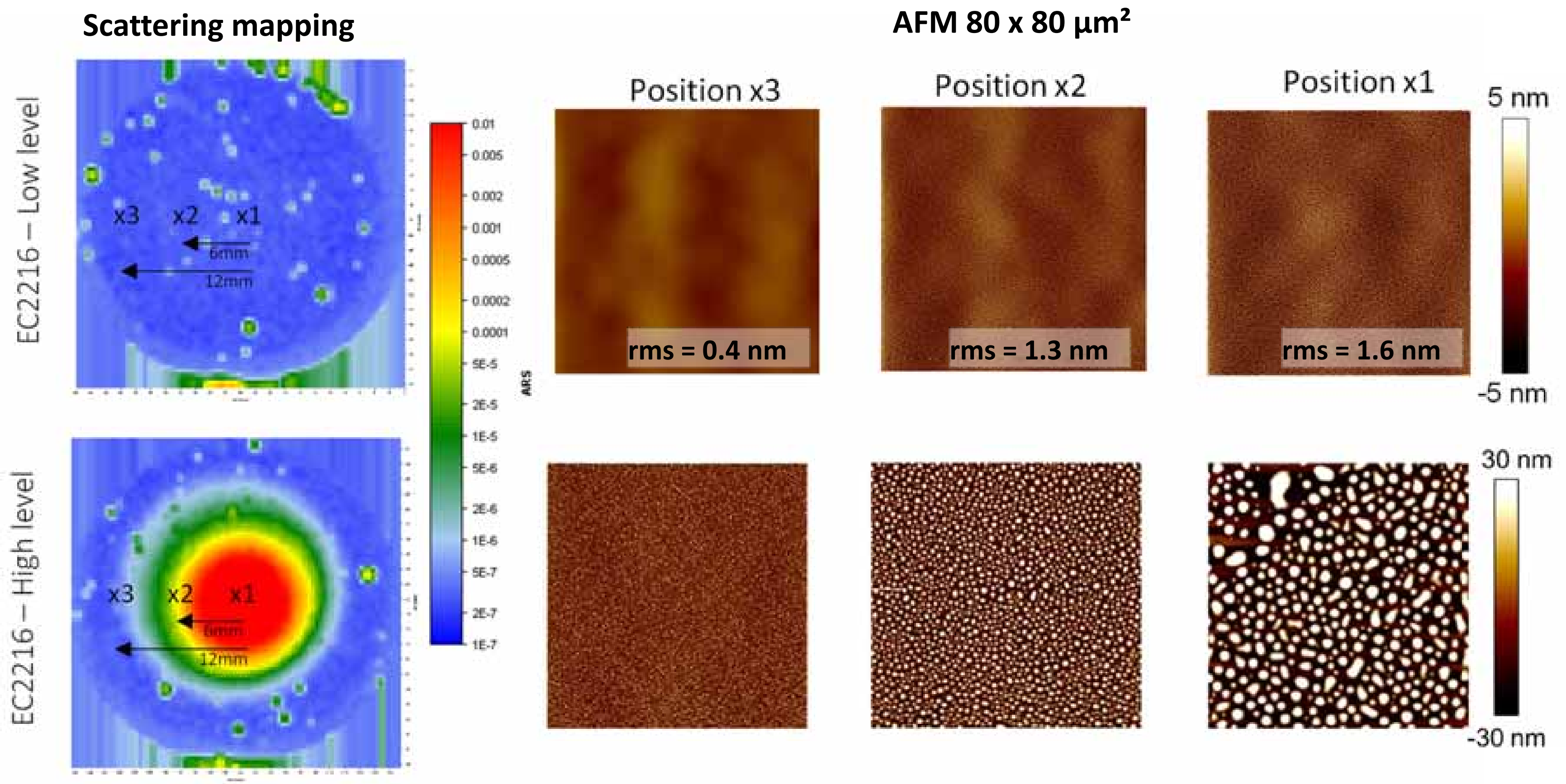




OHB Fraunhofer IOF

MOC - EC2216 on Si Wafer

topography



Ellipsometry / AFM

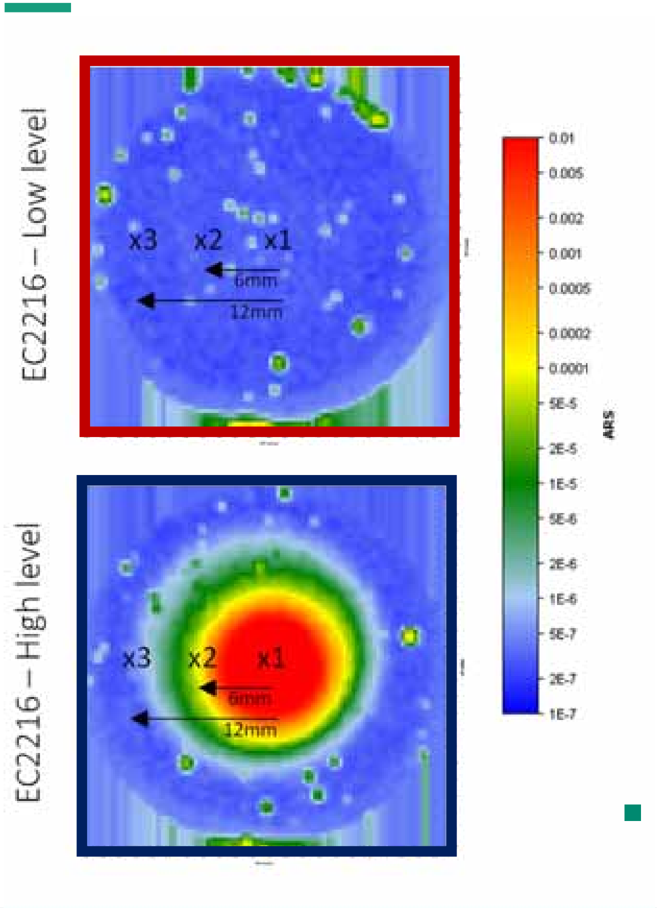
- **Thin Film** thickness:
  2 … 6 nm
- MOC level:
  200 … 650 ng/cm²

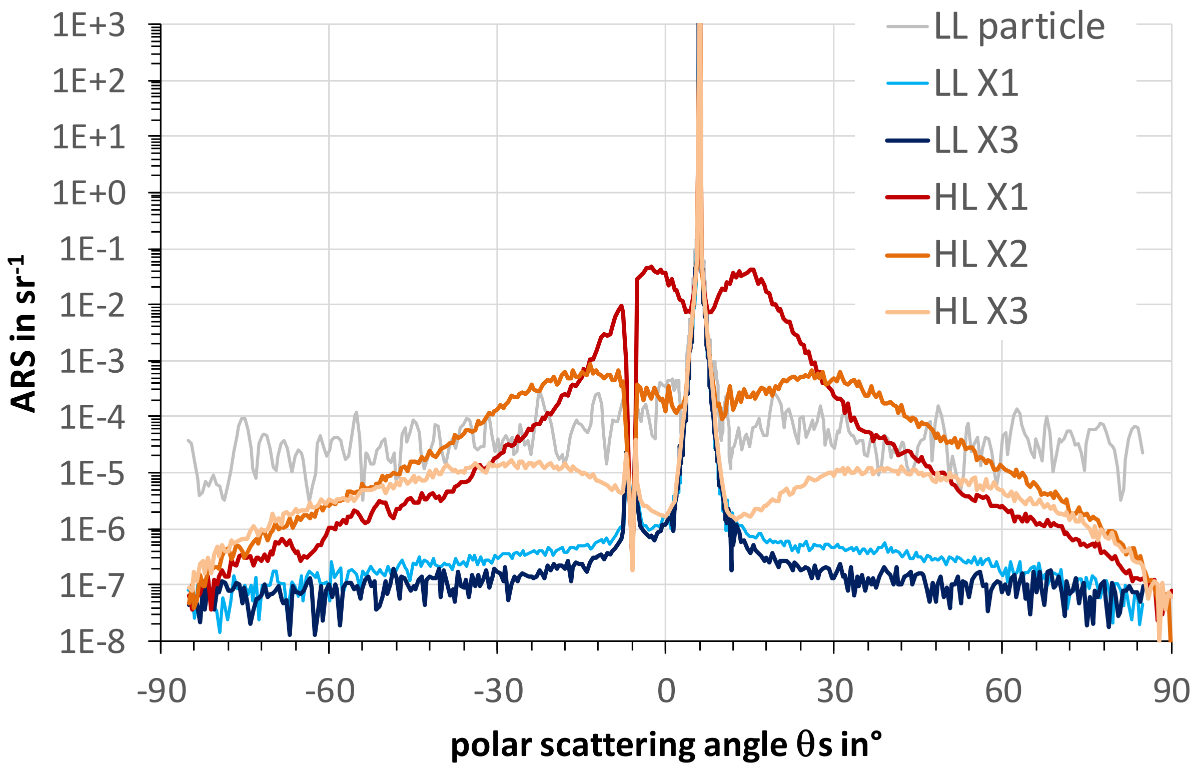
- **Droplets:**
  up to Ø6µm x H50nm
- MOC level:
  up to 3400 ng/cm²

OHB Fraunhofer IOF

MOC - EC2216 on Si Wafer

Scattering





- Minor effects or increase of scattering by **Factor >10^4**

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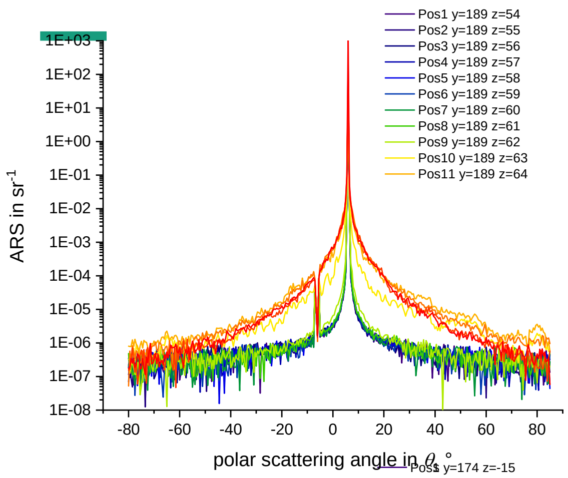
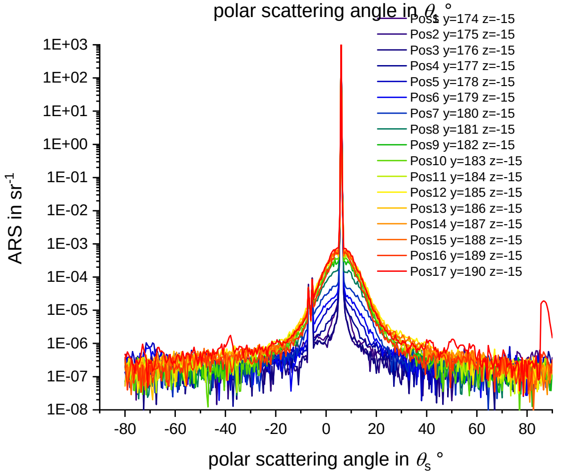
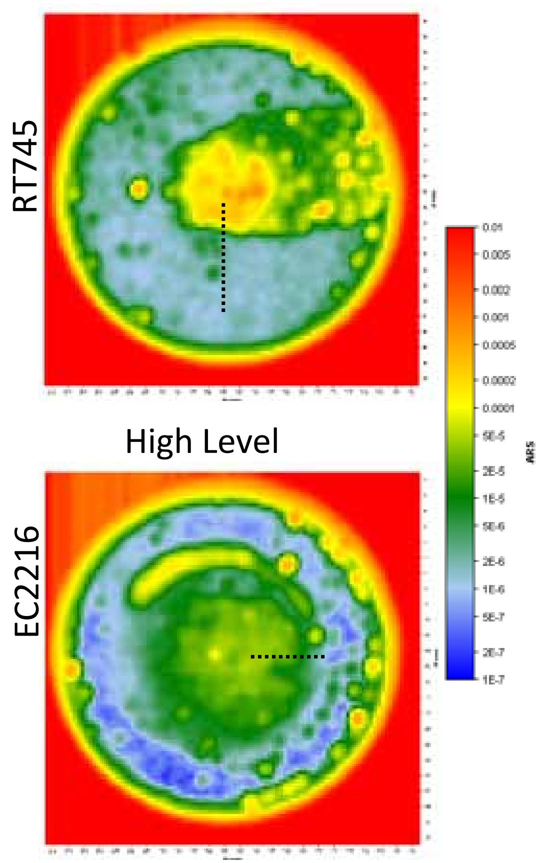
Analysis of MOC contamination – KG5 1064nm



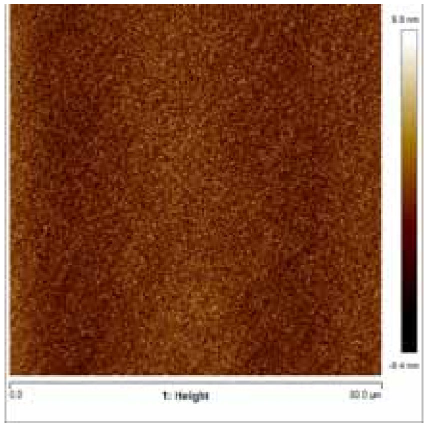


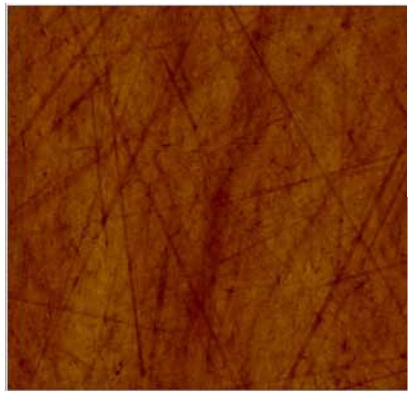
Low Level

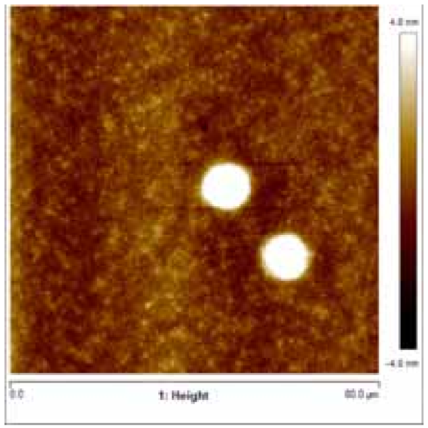
High Level



AFM 80x80µm²







- Significant differences between RT745 and EC2216 in BRDF & topography

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MOC

Summary

			Scattering mapping			Topography analysis		
contaminant	Envisaged level	substrate	Homogeneous haze	particles	clean	droplets	roughness	other
RT745	LL, 250ng/cm²	SiA		(x)	(x)		-	
		Si		x		(x)	increased	
		KG5	x				increased	No polishing features
	HL, 500ng/cm²	SiA			x		-	
		Si		x			-	
		KG5		(x)	(x)		-	Polishing features (+fine spikes)
EC2216	LL, 250ng/cm²	SiA	(x)		(x)		sign. changed inhomogeneous	
		Si	x	x		x	sign. changed inhomogeneous	
		KG5			(x)		slight increase	Polishing features still visible
	HL, 500ng/cm²	SiA	x			x		
		Si	x			x		Different from other droplets
		KG5	x			x	changed	(Big droplets)

- Inhomogeneous MOC density on surface from effusion cell
- MOC levels from ~0 to 3450e-7 g/cm²
- Thin film MOC between 100 ng/cm² to 640 ng/cm² analyzed

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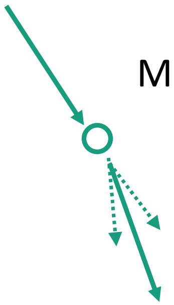
Agenda / Outline

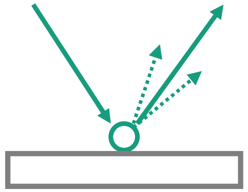
Modelling

- PAC scattering

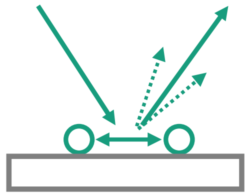
Mie Model – double interaction



MIE



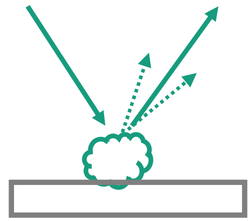
MIE based+ surface: Bobbert-Vlieger*
Double interaction *
+ many others



interference?

Rigorous
(FDTD or RCWA)

→ More oscillation
→ Not relevant (stochastic)



Particle form

Rigorous
(FDTD)

→ Not relevant (stochastic)

- Several theories reviewed and discussed
- Bobbert-Vlieger shall be exact for (MIE-)particles on surfaces (but, no particles >5µm possible …)
- MIE + Double interaction: Free space Mie particles + surface interaction (phase correct)

Thomas A. Germer, "pySCATMECH: a Python interface to the SCATMECH library of scattering codes," Proc. SPIE 11485,, 114850J (2020)

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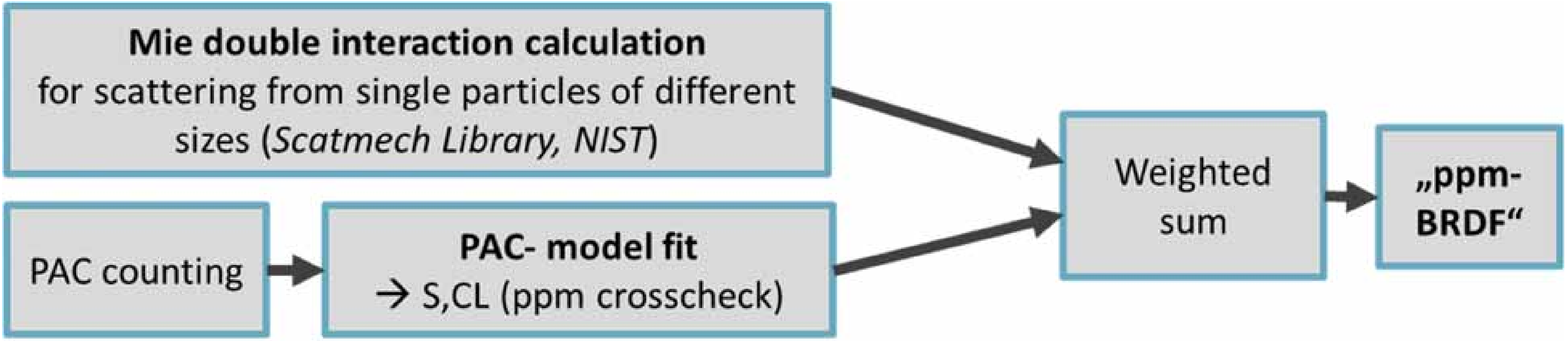
BSDF modelling

Summary of approach

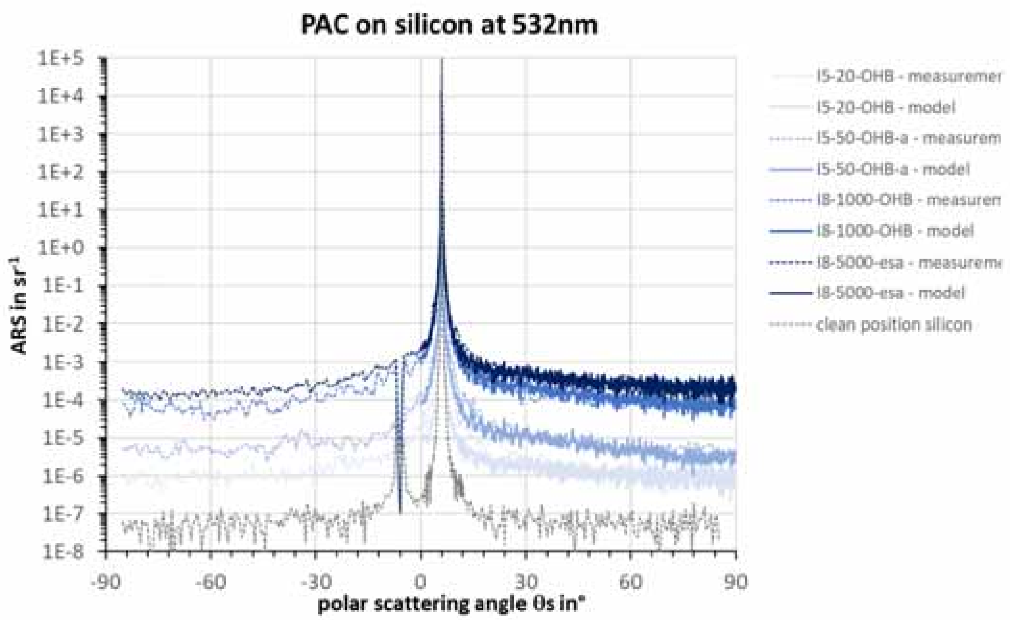


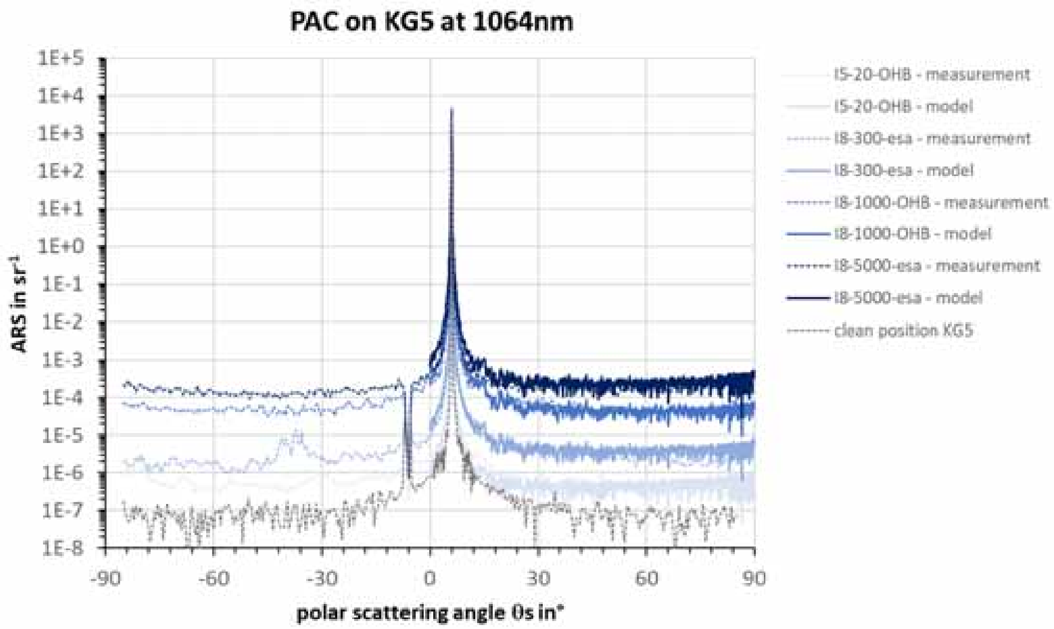
- Good Fit for different ppm-levels
- No significant wavelength scaling (big particles present)
- Good fit for measurements in transmittance
- Good fit of cleaned samples
- For low contamination levels single particles in duce stochastic uncertainty

Thomas A. Germer, "pySCATMECH: a Python interface to the SCATMECH library of scattering codes,"
Proc. SPIE 11485,, 114850J (2020)

BSDF modelling

General correlation

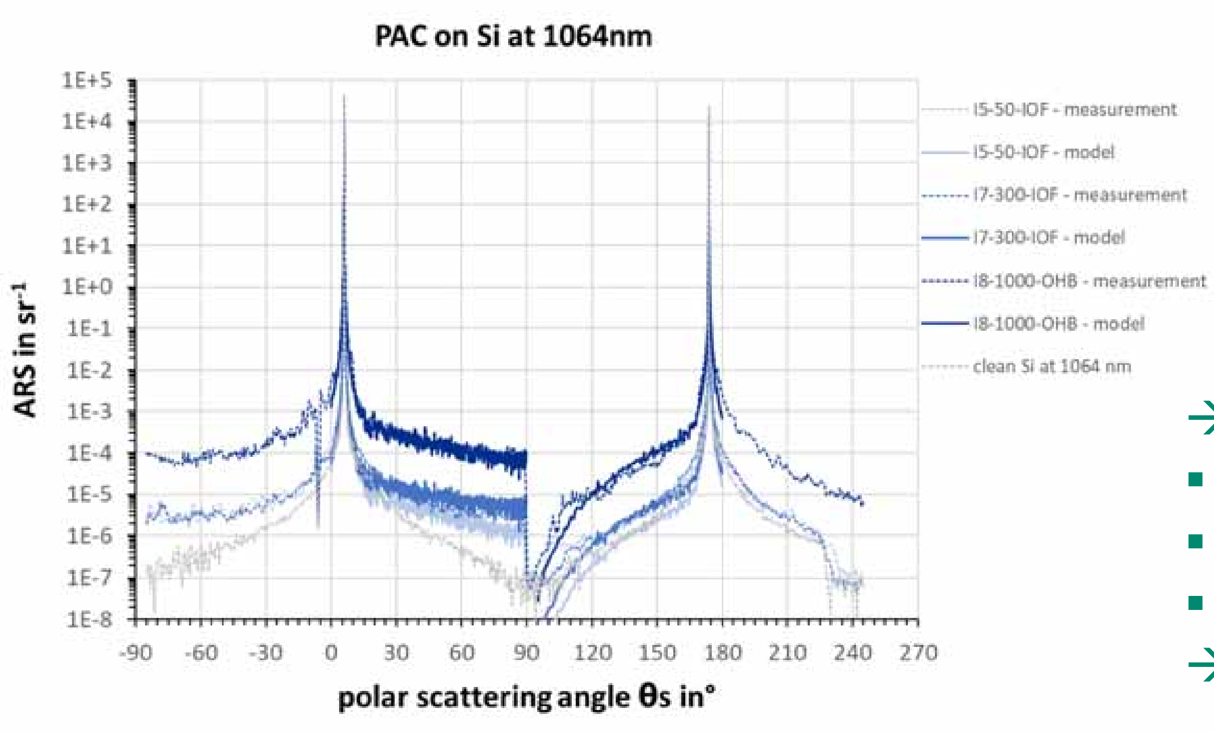


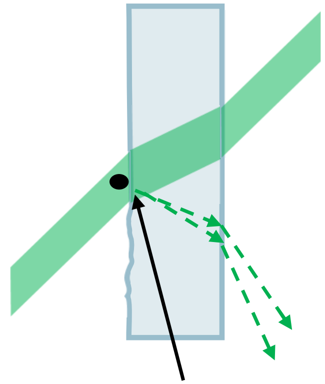


- Very good correlation for the selected samples

BSDF modelling

Transparent samples





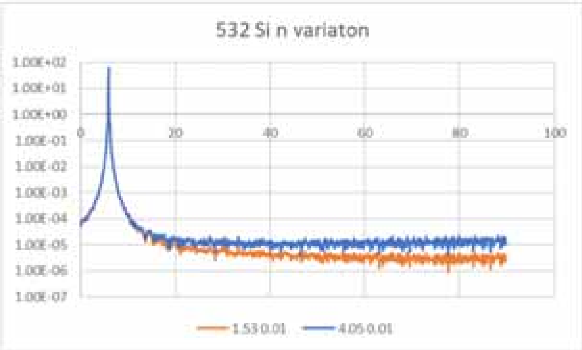
→ **BTDF results of ScatMech has to be modified:**

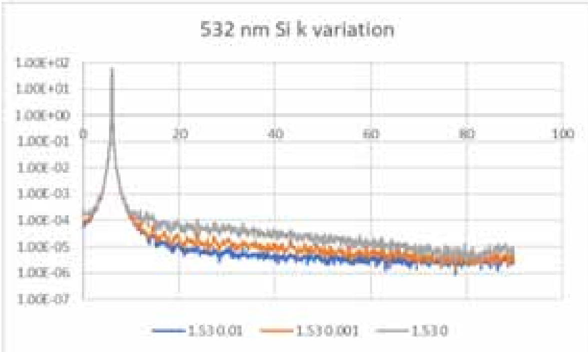
- Transmission through bulk & 2nd interface
- Refraction at 2nd interface
- Additional “diffraction” of solid angle

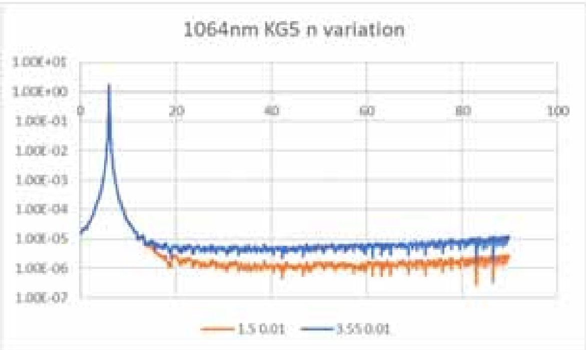
→ high contribution to slope at higher BTDF scattering angles

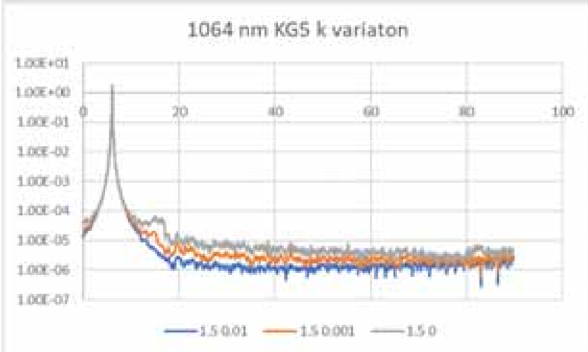
BSDF modelling

Influence of particle refractive index n/k









- Analyzing these influences on scattering + comparison to measured data
- Average refractive indices set to:

→ n = 1.53 + i0.001 @ 532nm

→ n = 1.50 + i0.001 @ 1064nm

- cross check to published values: almost same values as in literature or in FRED

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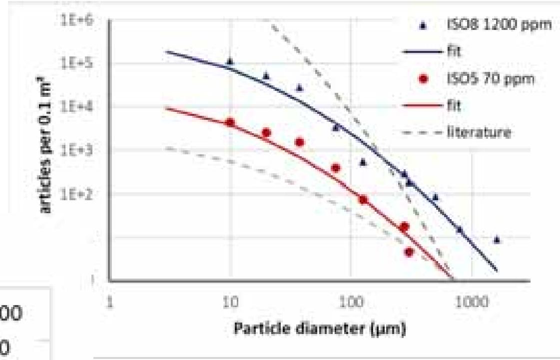
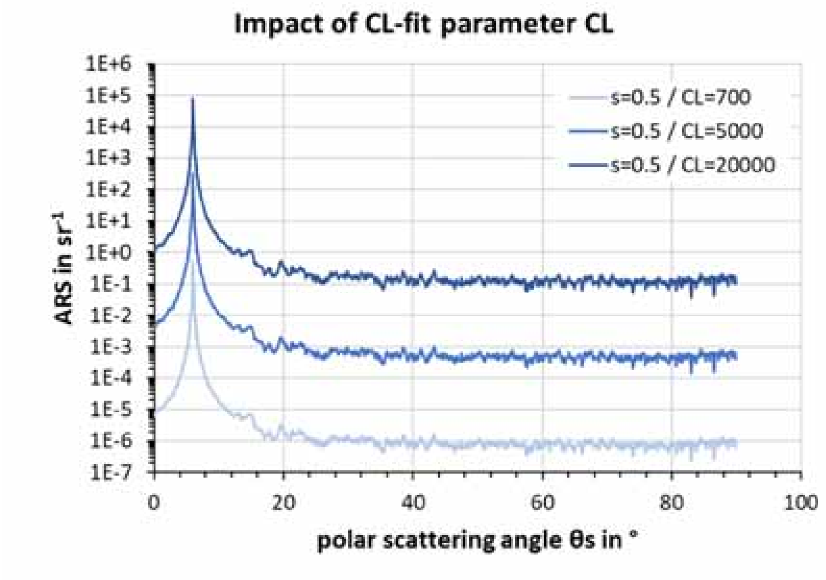
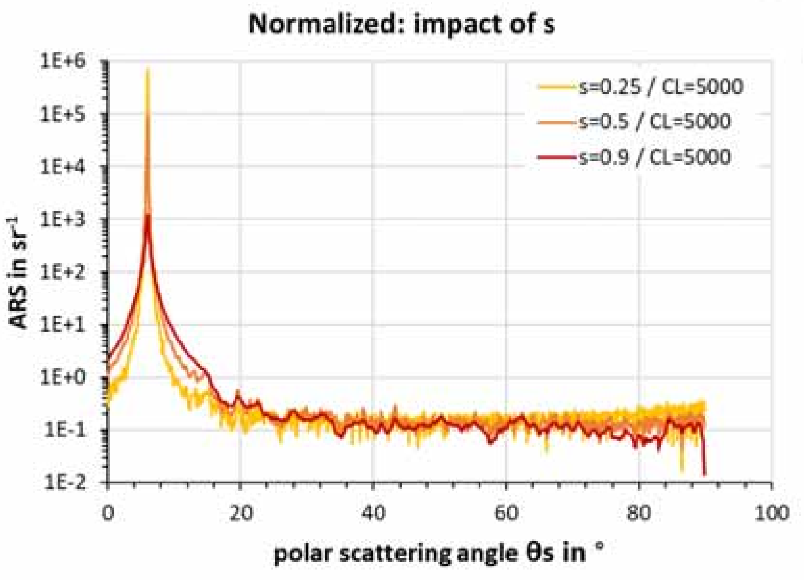
BSDF modelling

Influence of particle distribution (CL, s)







- Cleanliness Level: acts as global scaling factor
- Slope: also influences the global level (ARS normalized for comparison)

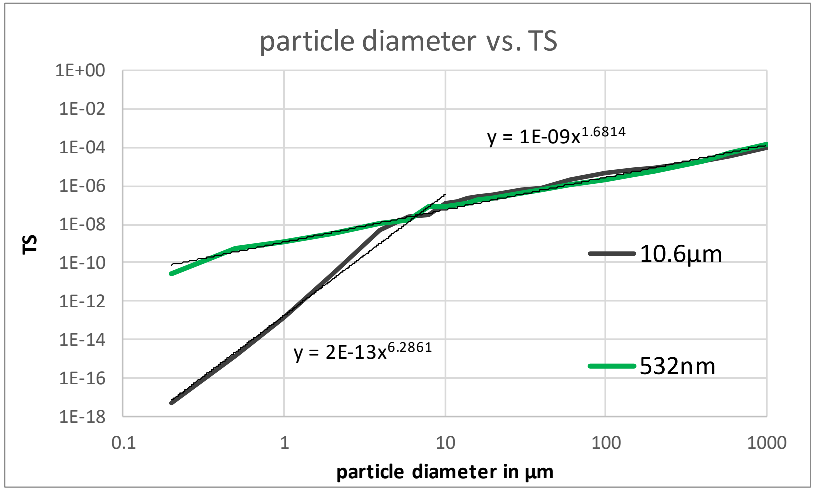
→ Moderate changes of scattering slope by particle distribution slope

→ observed slopes between 0.25 and 0.6 (0.7)

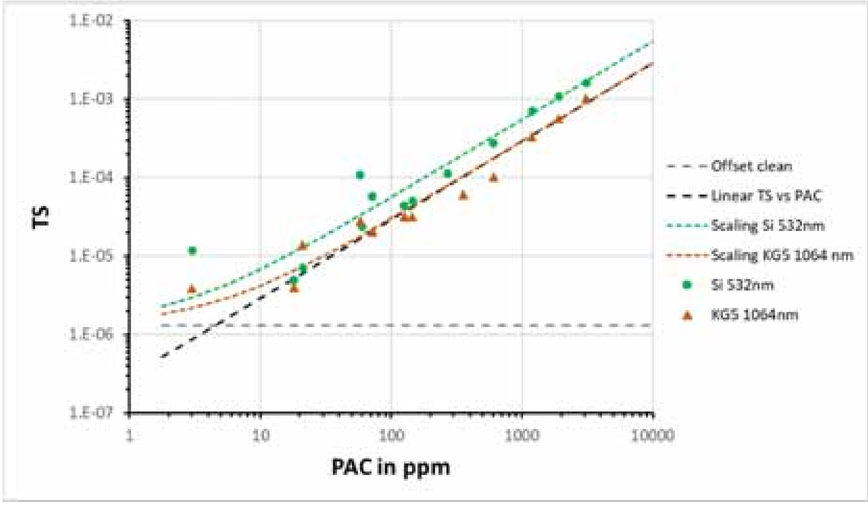
BSDF modelling

Contribution of particle sizes

Integrated scattering of single particles (model)



Integrated scattering vs. (experiment)

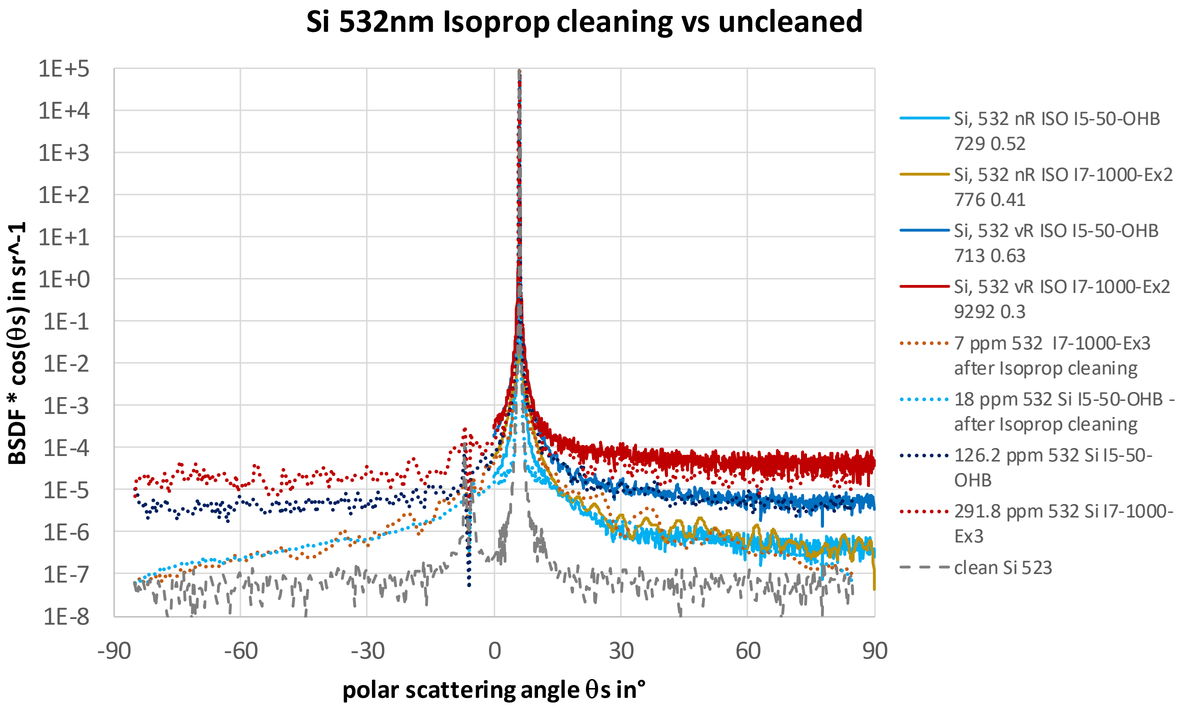


- integrated scattering (TS) of single according to power laws
- Different slope for diameter < or > λ

- In particular for high PAC almost linear growth of integrated scattering (TS) wit PAC

BSDF modelling

Influence of cleaning



- So far, no significant influence of particles with D <~ 5 µm observed

→ few big particles dominate BSDF

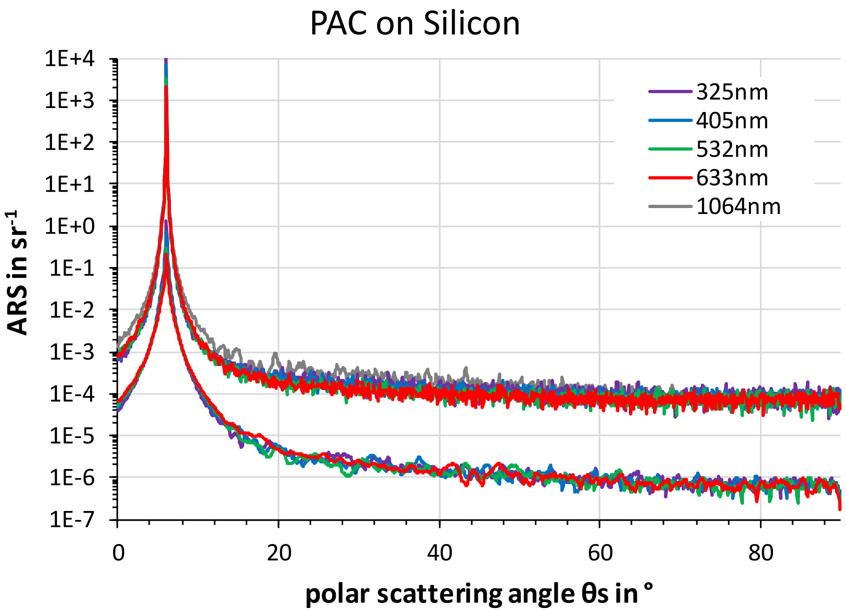
- After Isopropanol wiping a lot of small particles with D < 4µm observed

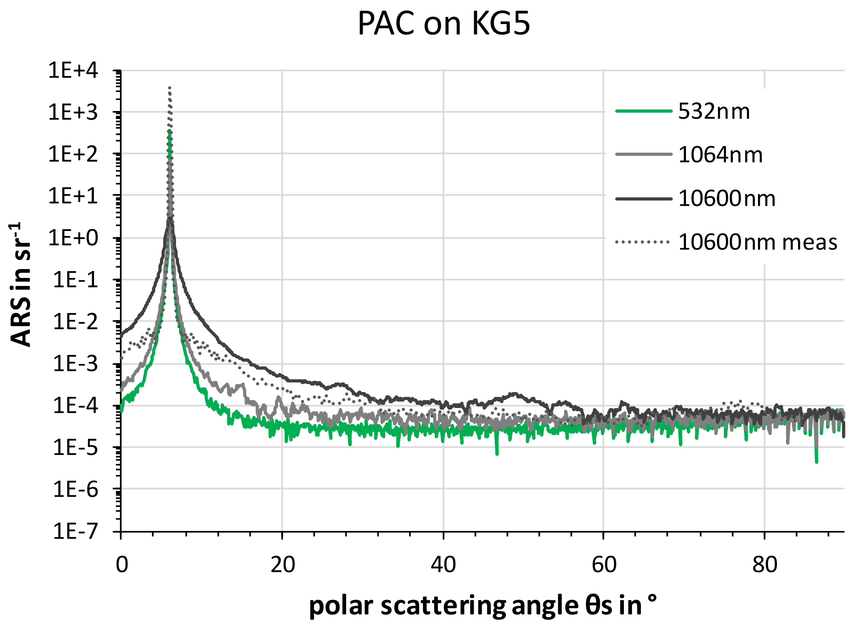
→ BSDF model fits only by including this exaggeration of small particles into particle distribution

→ CL-s PAC model not useful to describe this PAC distribution!

BSDF modelling

Wavelength scaling





- Model also predict sno significant wavelength scaling for VIS / NIR
- Increased near angle scattering for IR wavelengths

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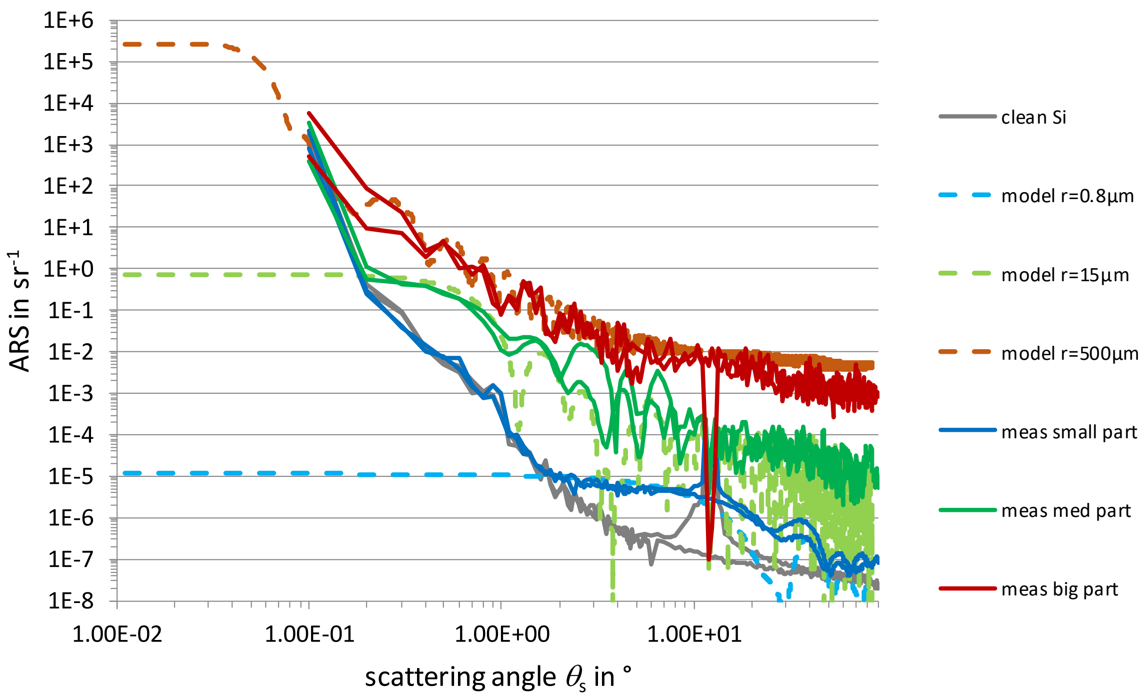
BSDF modelling

Wavelength scaling



- Comparison of scattering measurement and model for single particles

→ Particle scattering (meas & mod) intersects measured ARS (roughness induced/instrument signature) horizontally

→ Particle model continues horizontally until specular direction

→ **Particle scattering is not contributing to near angle scattering beyond this plateau**

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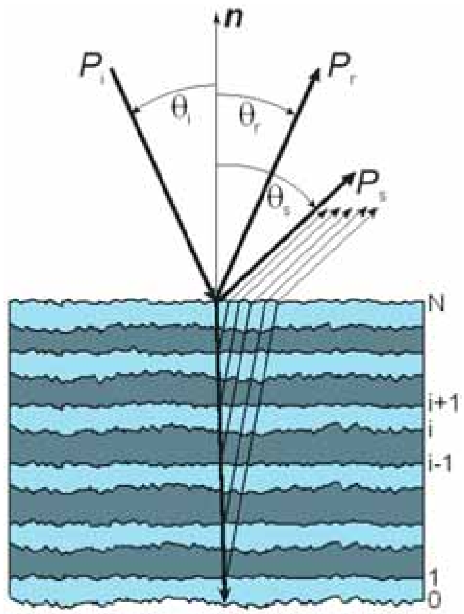
Agenda / Outline

Modelling

- MOC scattering

Scattering modelling from MOC

Thin film coating approach



Vector perturbation theory (σ << λ)

$$ARS(\theta_s) \sim \frac{1}{\lambda^4} \sum_{i=0}^{N} \sum_{j=0}^{N} F_i F_j^* \, PSD_{ij}(f)$$

Optical factors

- Multilayer design
- Optical constants
- Polarization

Roughness factors

- PSDs of individual surfaces
- Cross-correlation properties (i≠*j*)

PSD: Power Spectral Density of surface roughness
(~ Fourier Transform)

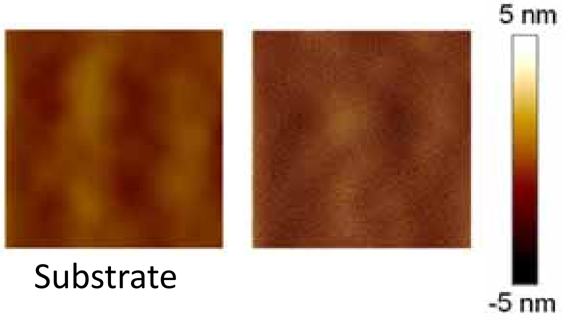
- Multilayer scatter influenced by roughness and interference effects
- **Application for a single thin MOC layer on Si/KG5 substrates ?**
- **PSD + Film parameters of MOC ?**

J. M. Elson et al., Appl. Opt. 19, 669-679 (1980)
P. Bousquet et al., J. Opt. Soc. Am. 71, 1115-1123 (1981)

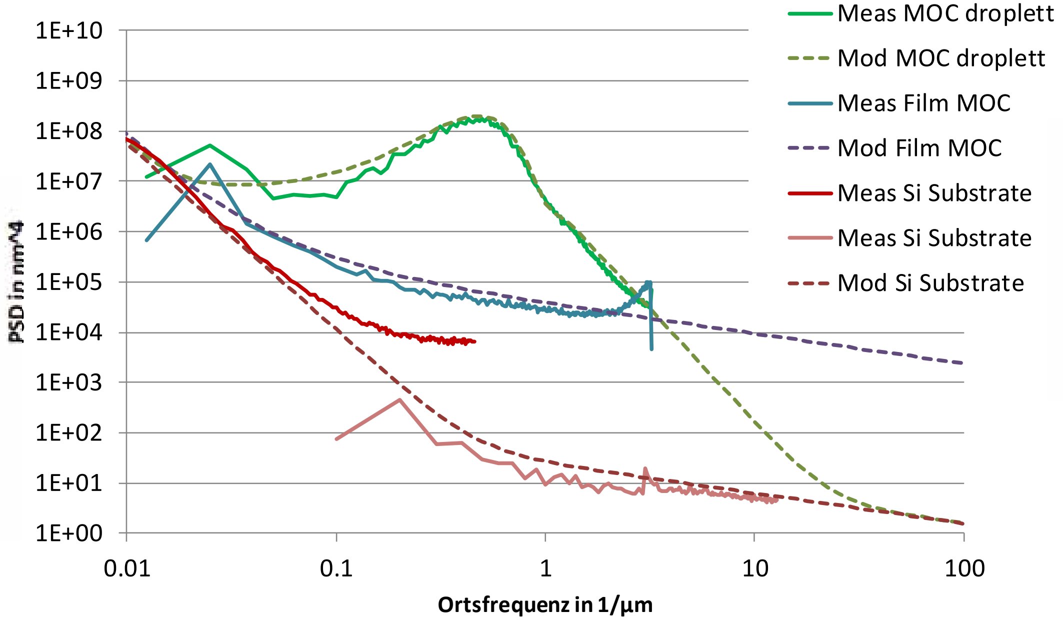
Scattering modelling from MOC

"Roughness" of MOC

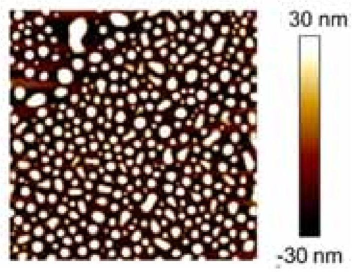
Thin film MOC on Si



Substrate



Droplet MOC on Si

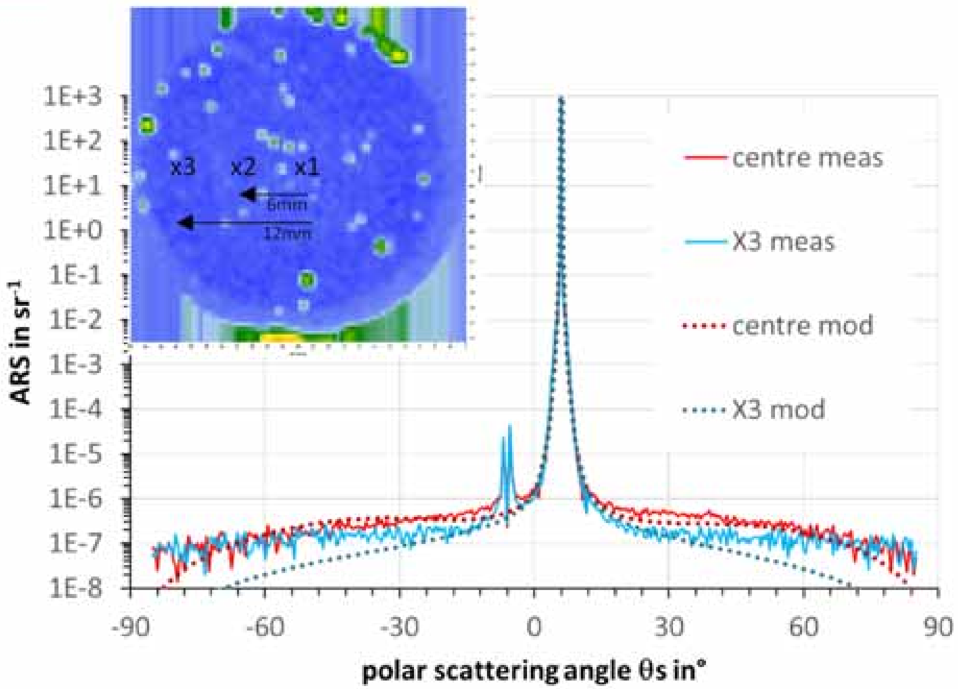


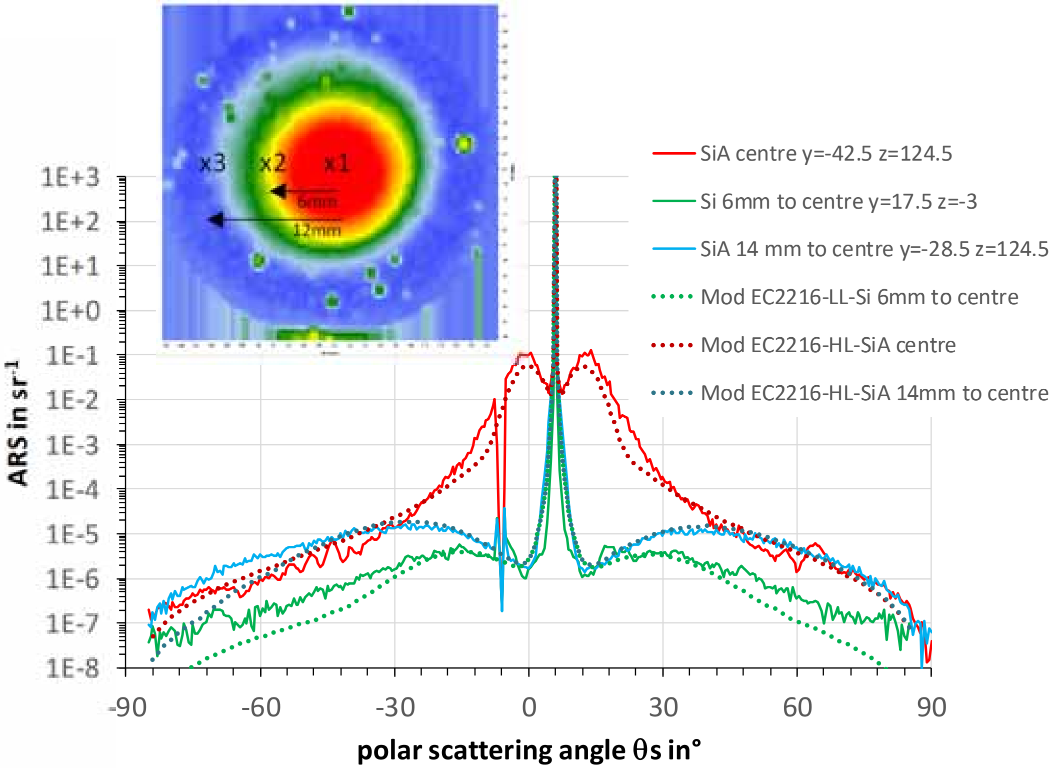
- AFM topography data → PSD (model function)
- n, k from tables
- Film thickness from Ellipsometry

- AFM topography data → PSD (model function)
- n, k from tables
- Thickness → „effective thickness" from geometry ~ 1/3 of droplet height

Scattering modelling from MOC

Results: EC2216 on Si





- Modelling: Thin Film scattering theory gives excellent results for thin film & droplet MOC

P. Bousquet, et. al, “Scattering from multilayer …,” J. Opt. Soc. Am. 71 (1981);
S. Schröder, T. Herffurth, et al., “Angle-resolved scattering: an effective method for characterizing thin-film coatings,” Appl. Opt. 50 (2011);
T. Herffurth, “Roughness and optical losses of rugate coatings,” Appl. Opt. 53 (2014).

Agenda / Outline

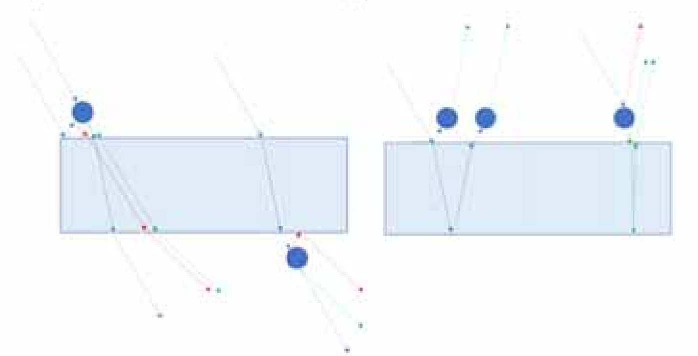
Modelling
- System level

Modelling on system level

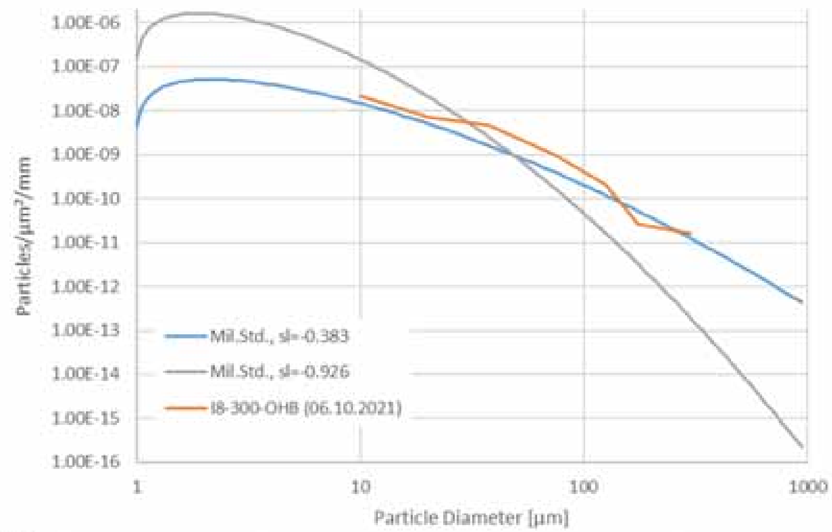
BSDF models into Ray-Tracing Software

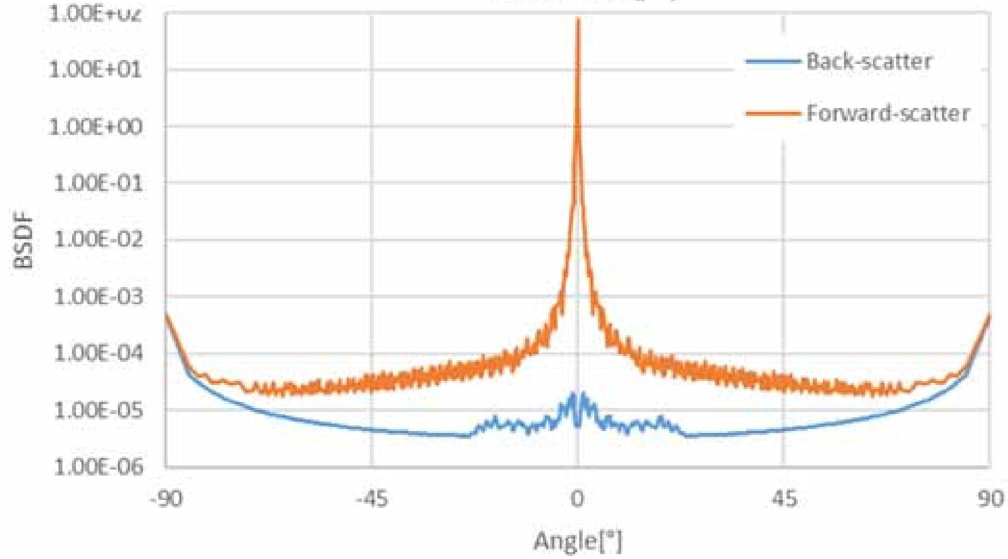
Software FRED:

- MIE model implemented including particle distributions according to MIL-STD-1246C
- "double interaction" implicitly implemented
  → particle scattering interacts with surface



- Implementation of customized scattering models or import of external modelling data supported





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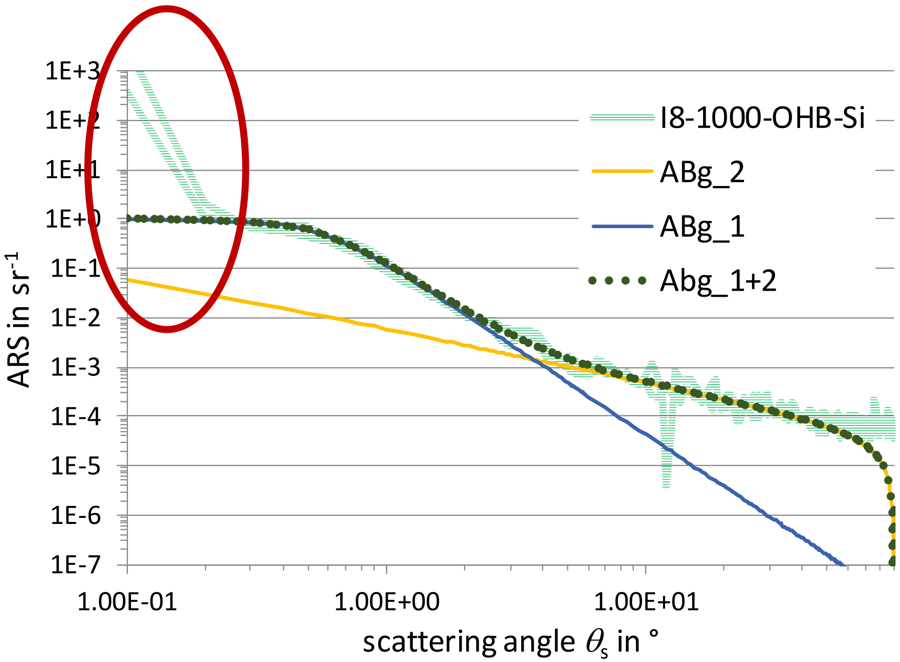
Modelling on system level

BSDF import into Ray-Tracing Software

n	A	B	g
1	7e-5	3e-4	1.1
2	9.5e-8	1e-7	3.5

$$ARS = \cos\theta_s \sum_{n=1}^{2} \frac{A_n}{B_n + |\sin\theta_s - \sin\theta_i|^{g_n}}$$

- **Direct import** of measured data
- Fitting of measured curves with **ABg model** e.g. with two terms:
  → less oscillation / "noise"
  → However, poor fit at high scattering angles (reducible by 3rd term or use θ_s instead of $\sin\theta_s$)
- Proposal for handling of near angle scattering: **horizontal plateau** since near angle scattering is not driven by particles
- FRED will handle transmittance, reflectance, refraction, … of this data
  → **care required not to consider those effects twice**



Modelling on system level

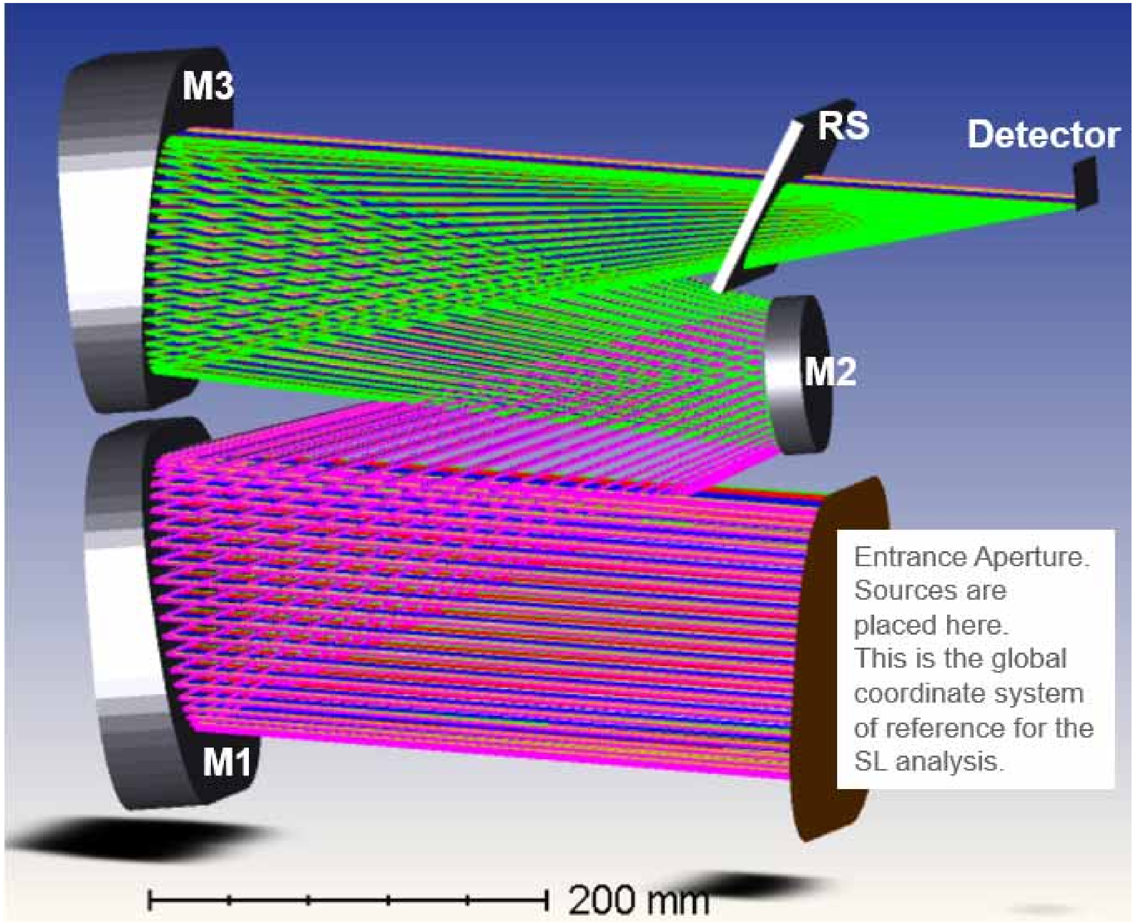
Optical system

- Test system: TMA imaging system, VIS:
  EFL= 545 mm
  F# = 4
  FoV = +/-2.91 °

- Three mirrors (M1,M2,M3)
  one refractive element/window (RS)
  and Detector.

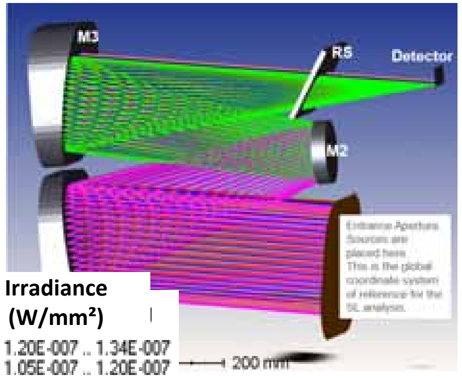
- Measured BRDF data applied for PAC

- Modelled for:
  Half Field Illumination → contrast degradation
  Punctual Illumination → PSF degradation



Modelling on system level

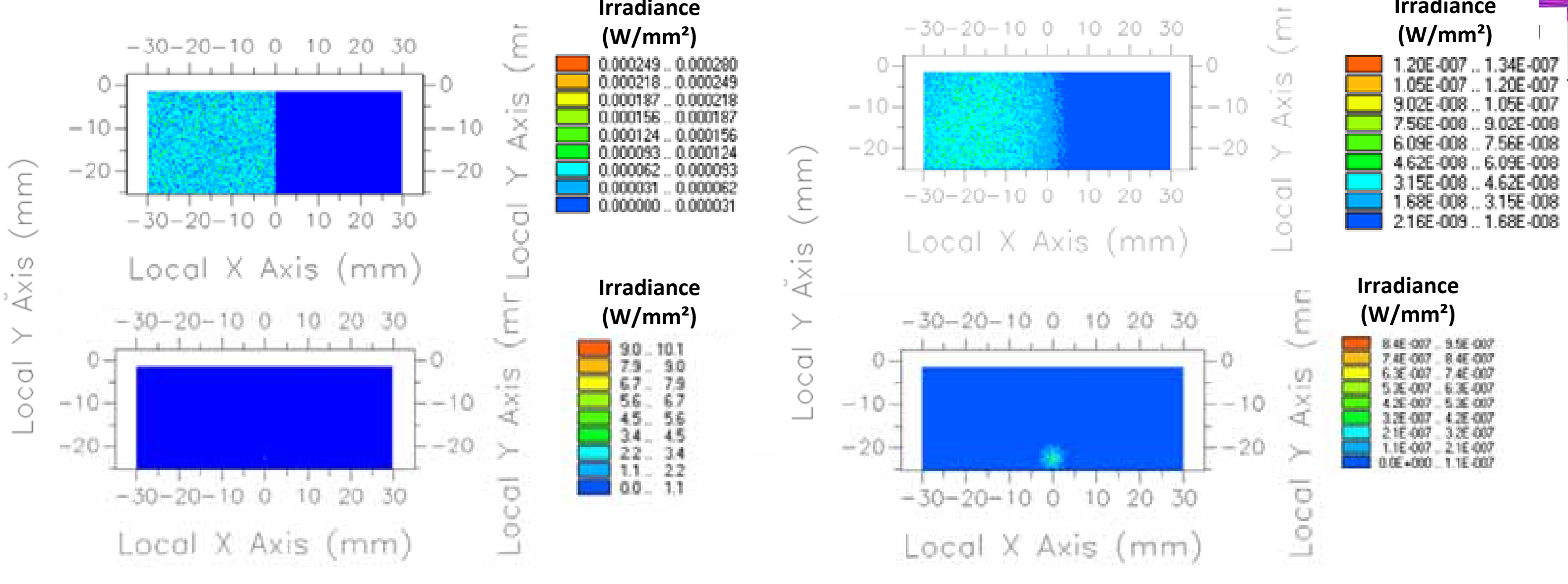
Influence of contamination



Direct light | **Scattered light**

Half field illumination

Point source



- Scattering contribution to bright field >3000x lower than direct light
- Scattering close to point source x10^{-7} lower than image of the point source

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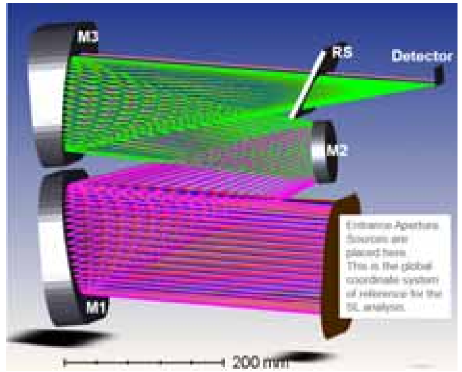
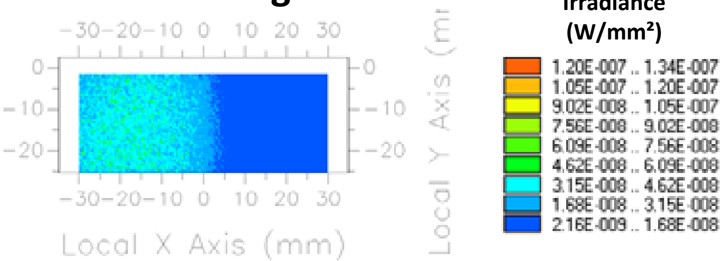
Modelling on system level

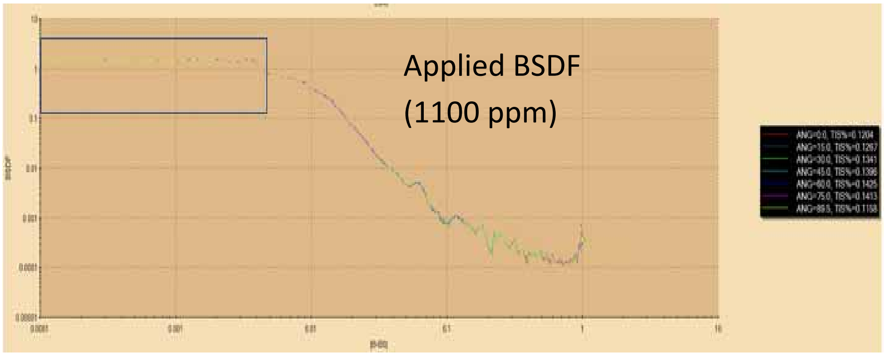
Influence on contrast

- Half field illumination normalized to direct light
- Vertical averaging to reduce noise

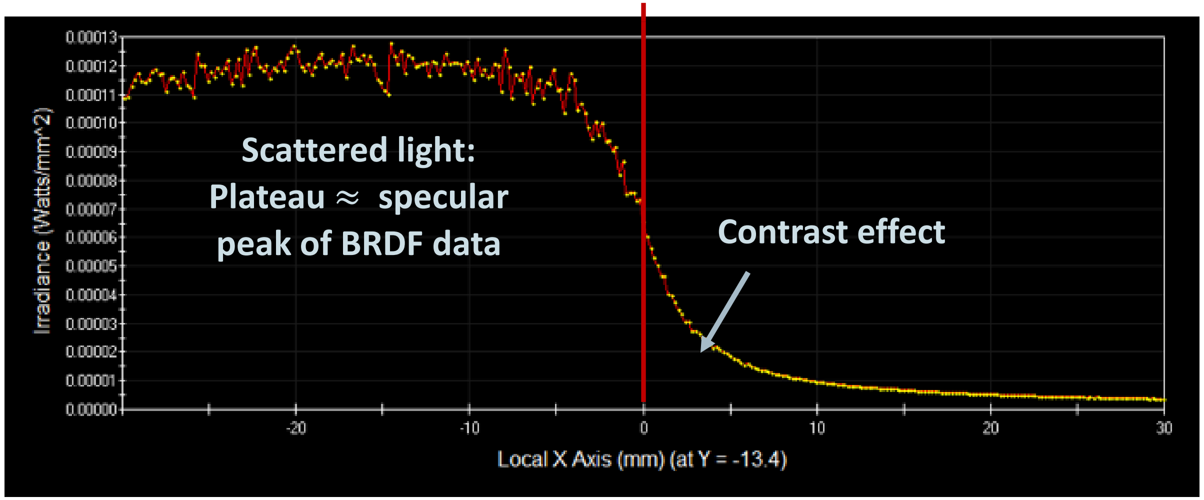


Scattered light

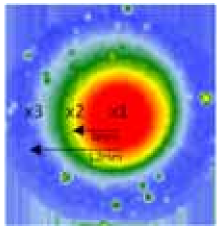


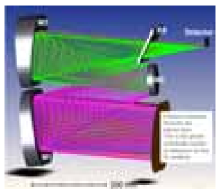


1 W/mm² (direct light)



Summary





- Light scattering from PAC & MOC is critical factor for optical coatings, components and systems → image degradation & losses
- **Project CoCis**: initiated by esa to obtain reliable & experimentally verified data & models for contamination induced scattering
- PAC collected by exposure in different clean rooms; MOC generated by effusion cell
- Results for real world scattering of PAC contaminated surface

  → Linear scaling of scattering according ppm
  → No significant wavelength scaling
  → Influence of optical properties of substrate
  → "Efficiency" of cleaning approaches
- MOC: forms as thin films or droplets with tremendous effect on scattering
- PAC modelling using MIE double interaction theory
- MOC modelling (thin films/droplets) using thin film techniques

Thank you for your attention

Thanks to colleagues:
Marius Wyltschew, Anna Gottwald, Nadja Felde, Marcus Trost, Anne-Sophie Munser, Sven Schröder (IOF)
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John Stover, Chris Staats (TSW); Thomas Germer (NIST); Mathilde Marcon (Thales)
Mircea Helici, Holger Fischer, Simon Strotman, Volker Kirschner (esa)
….