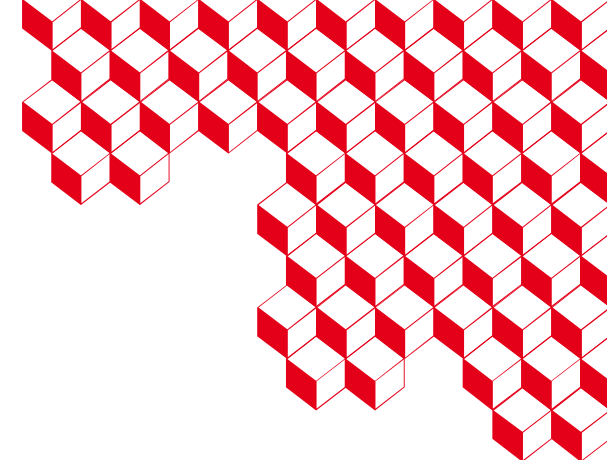




list



Development of a numerical X-ray imaging model for phase-contrast and dark-field imaging

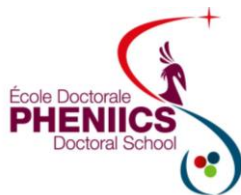
Youliana Mouawad

14 Novembre 2024 → 15 Novembre 2027

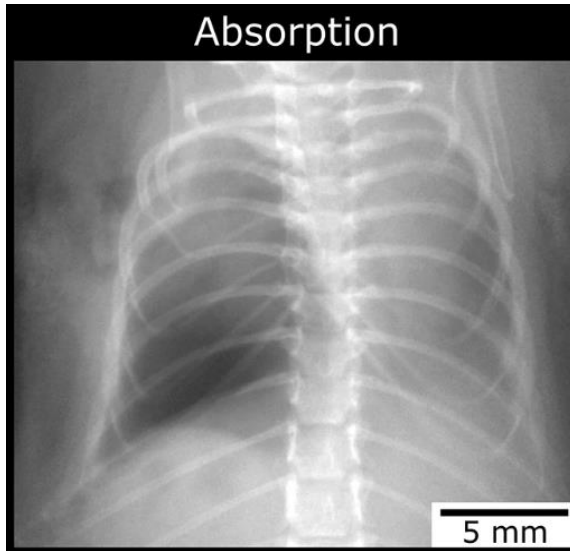
Director : Adrien Stolidi (DIN/SMCD/LIMTEC)

Supervisors : Anthony Tournon (DIN/SSIA/LSMA) & Juan Carlos García Hernández(DIN/SIMRI/LEMA)

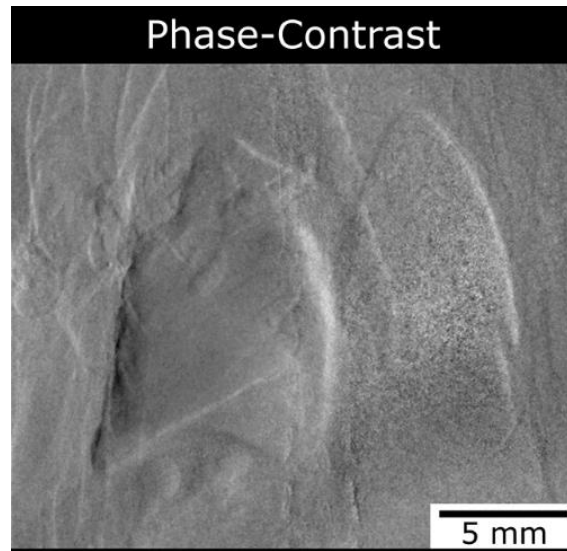
Funded by the Carnot OSIRIS project



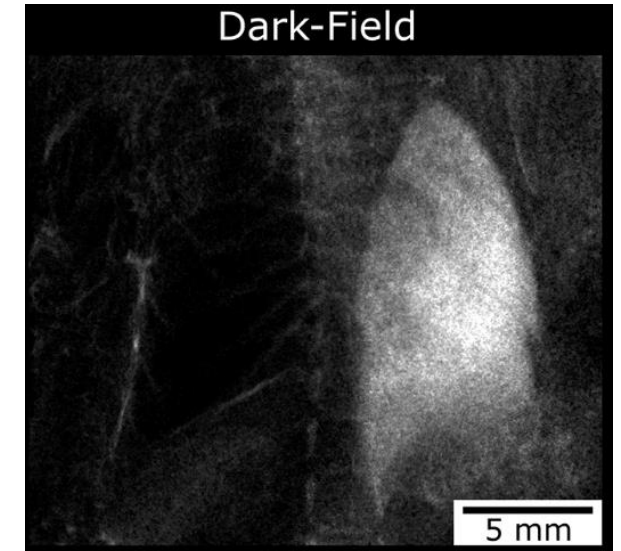
X-ray Imaging Methods



- Beam attenuation (Beer–Lambert law)
- **Low contrast** for **soft tissues**



- The object induces a phase shift in the wavefront
- The observed image mainly reflects the **phase gradient**
- **Enhanced contrast** for soft tissues



- Sensitive to **multiple small-angle scattering**
- Reveals **fine internal microstructure**



1 ■ Objectives

Objectives

Main objective: Design and validate a numerical simulator for phase-contrast and dark-field X-ray imaging, with the best trade-off between accuracy and computation time

➤ **Modeling approaches:**

Wave-based

Fresnel :

Interference
Phase shift
Scattering

Particle-based

Ray Tracing :

Interference
Refraction
Scattering

Monte Carlo :

Interference
Refraction
Scattering

Existing model in CIVA — Hybrid Fresnel

➤ CIVA environment:

- We rely on the existing tools of the imaging system
→ X-ray source, object geometry, detector
- **Why “hybrid”?**
- **Particle-based step — ray tracing**
→ ray launching
→ estimation of absorption and phase shift at the object exit
- **Wave-optics step — Fresnel**
→ propagation of the field to the detector

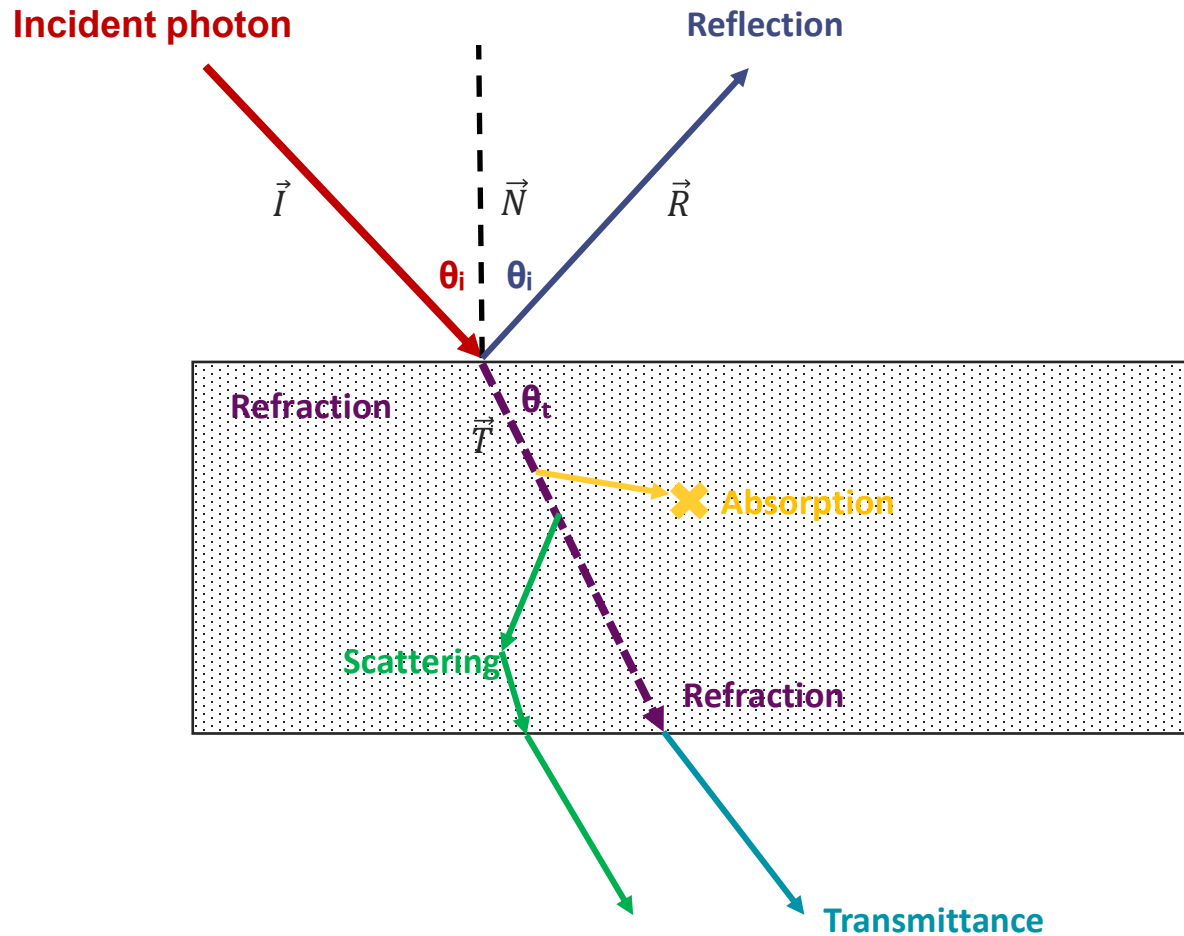
➤ Model limitations:

- Paraxial approximations: limited validity outside small-angle conditions
- Thin-object approximation: limitations for big samples
- Oversampling / pixel size: direct influence on the result
- Numerical errors: due to ray tracing



Developed model

CIVA – Developed Monte Carlo model (Refraction – Reflection)



Critical angle :

$$\Theta_c = \arcsin\left(\frac{n_1}{n_2}\right)$$

Cas 1 : Total Reflection $\theta_i > \theta_c$

Direction :

$$\vec{R} = \vec{I} - 2(\vec{I} \cdot \vec{N})\vec{N}$$

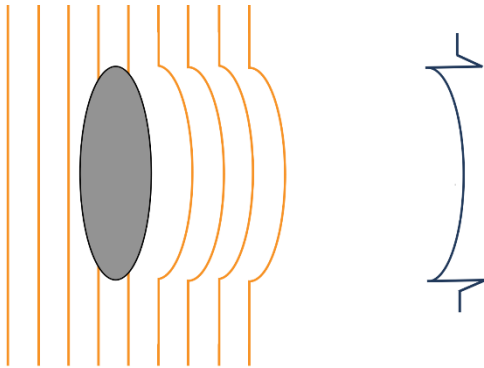
Cas 2 : Refraction

Direction :

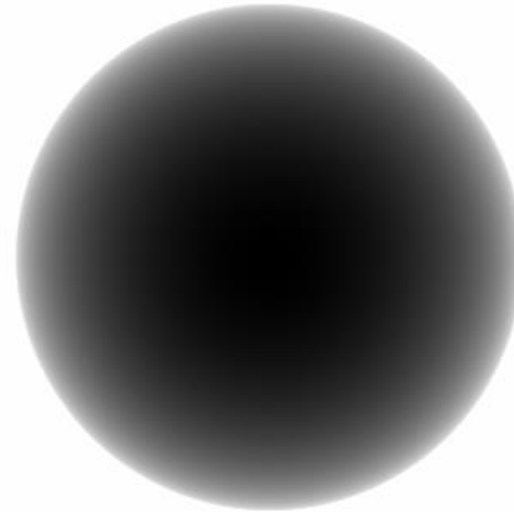
$$\vec{T} = \eta \vec{I} + (\eta \cos \theta_i - \cos \theta_t) \vec{N}$$

$$\text{avec } \eta = \frac{n_1}{n_2}$$

Application of the model to free-space propagation — Case study

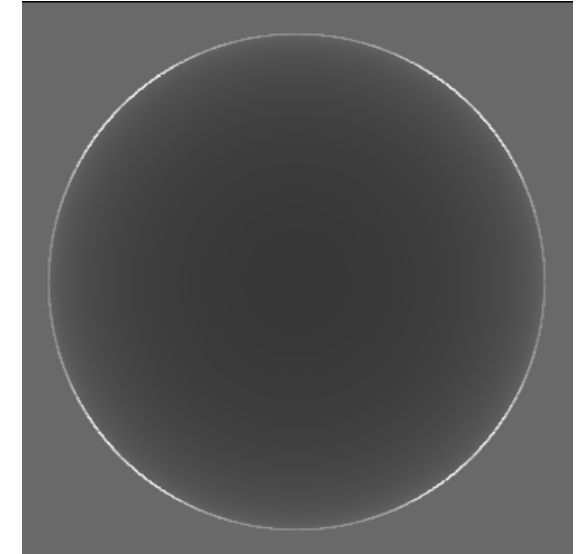


- Beam propagation in **free space**, without optics or gratings
- The **phase shifts** induced by the object are converted into **intensity variations** at the detector



Absorption image :

- No phase propagation



Phase image :

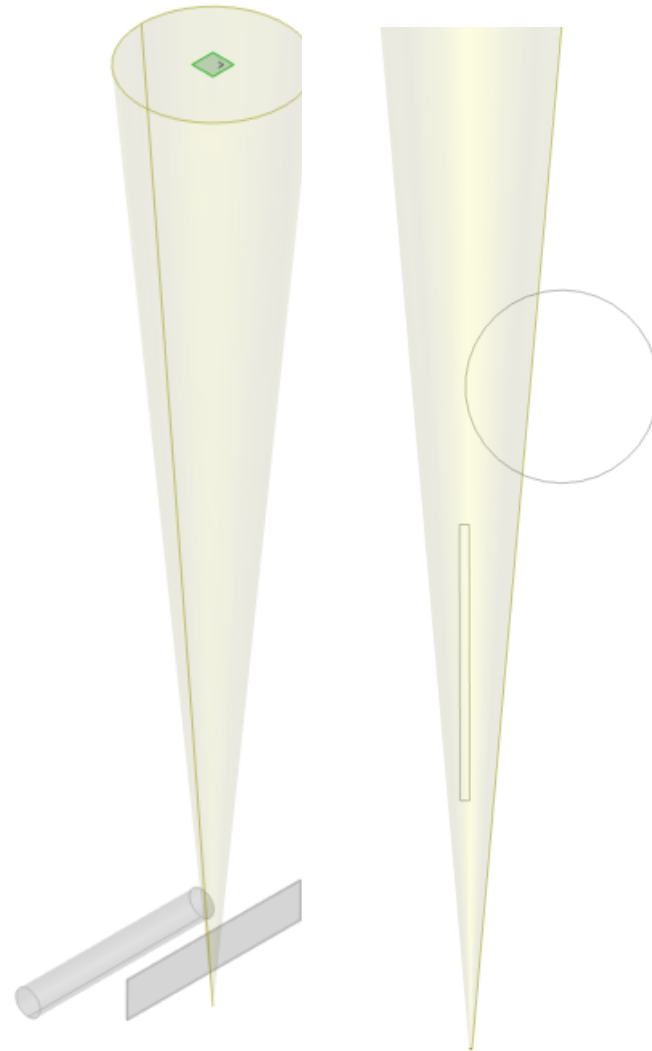
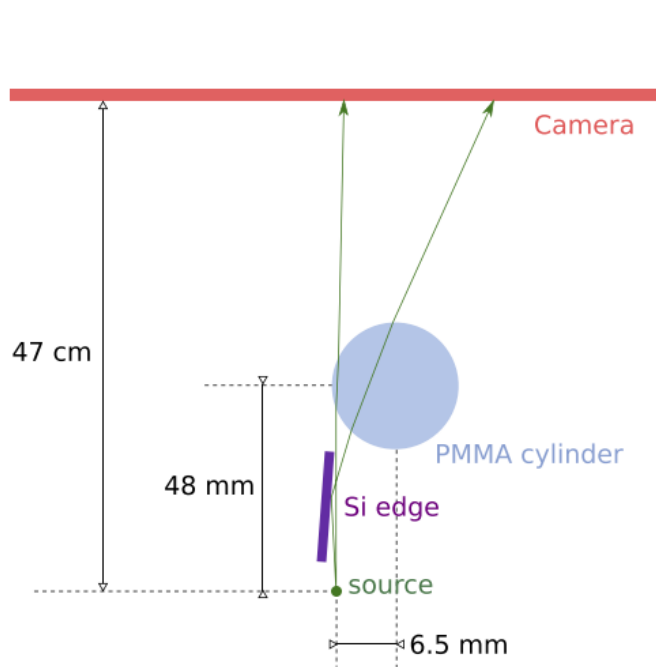
- Appearance of edge-enhancement



2 ■ Results

Comparison with other models from the literature

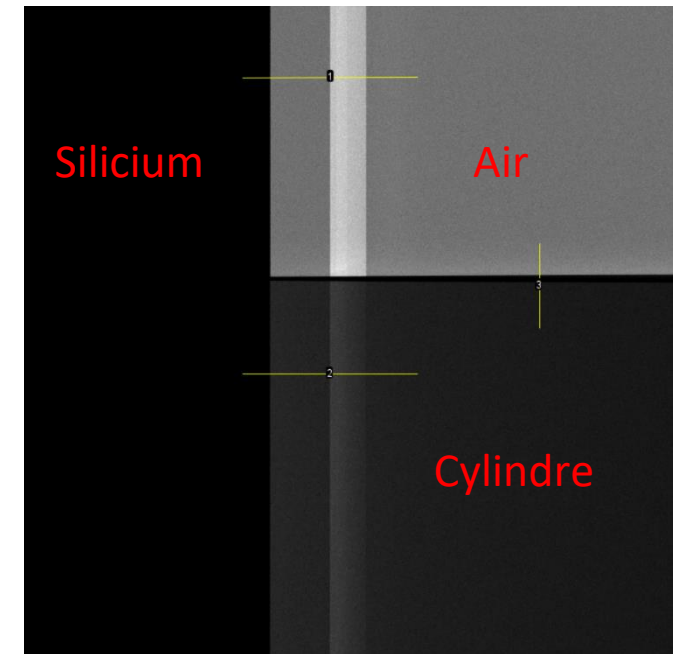
Silicon cylinder / edge – Comparison of CIVA MC refraction / Max Langer



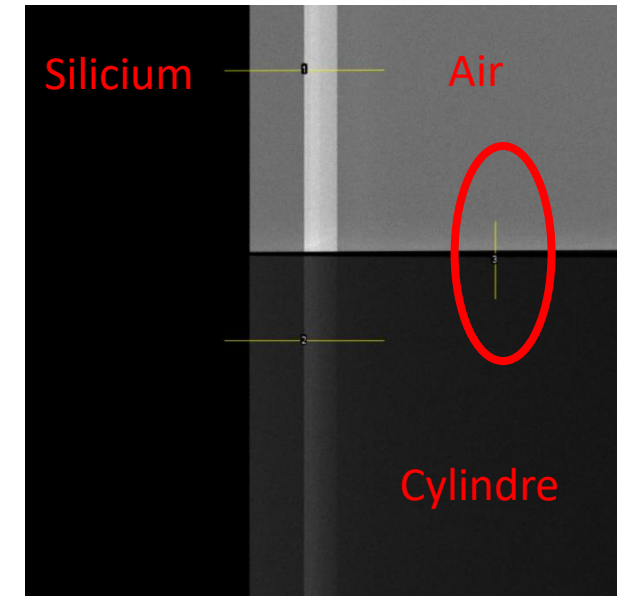
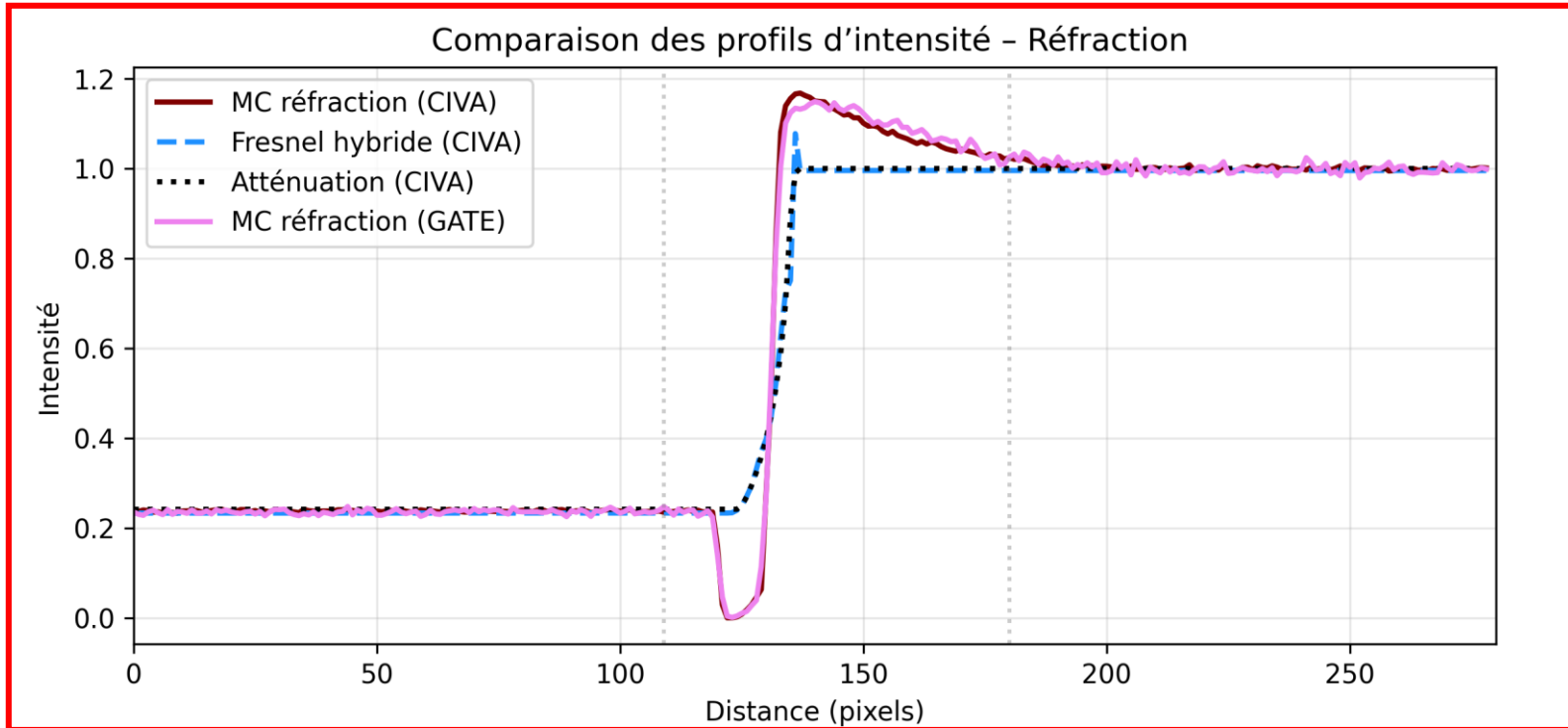
Towards Monte Carlo simulation of X-ray phase contrast using GATE

MAX LANGER, ZHENJIE CEN, SIMON RIT, AND JEAN M. LÉTANG*

University of Lyon, INSA-Lyon, Université Claude Bernard Lyon 1, UJM-Saint Etienne, CNRS, Inserm, CREATIS UMR 5220, U1206, F-69373 Lyon, France
*jean.letang@creatis.insa-lyon.fr

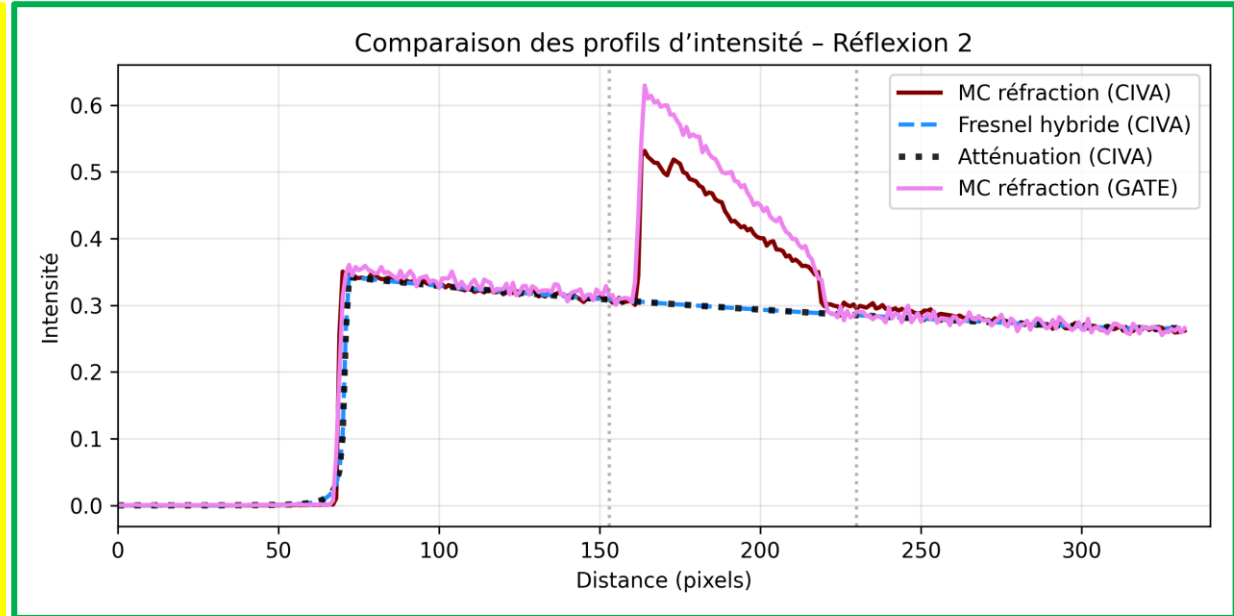
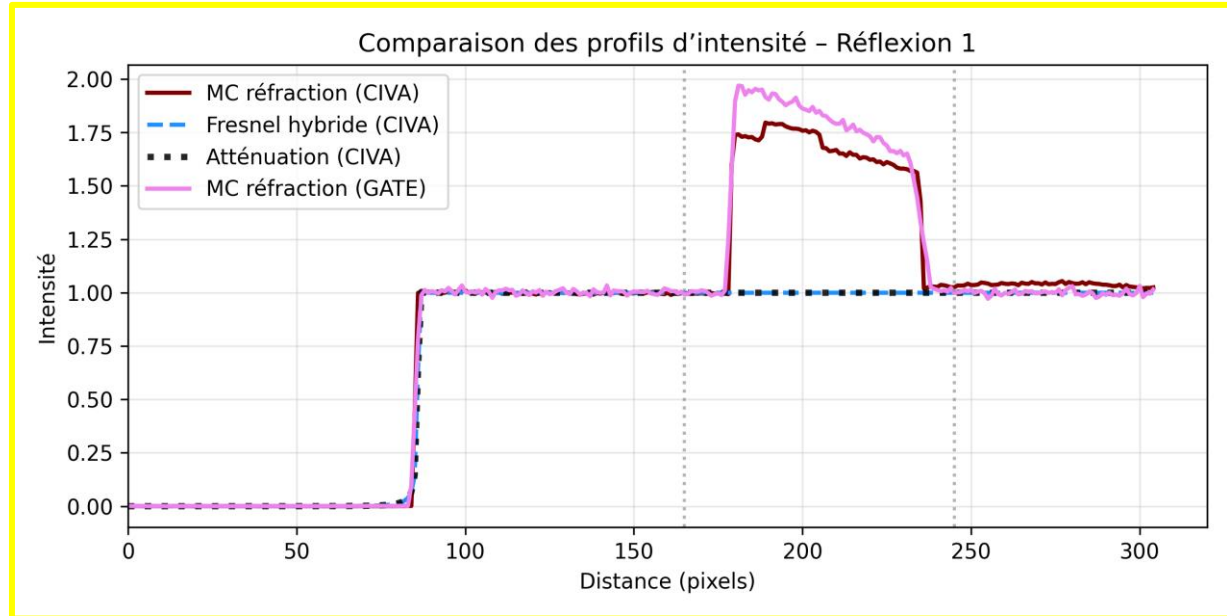


Refraction: MC refraction (CIVA) / Hybrid Fresnel (CIVA) / MC refraction (GATE)

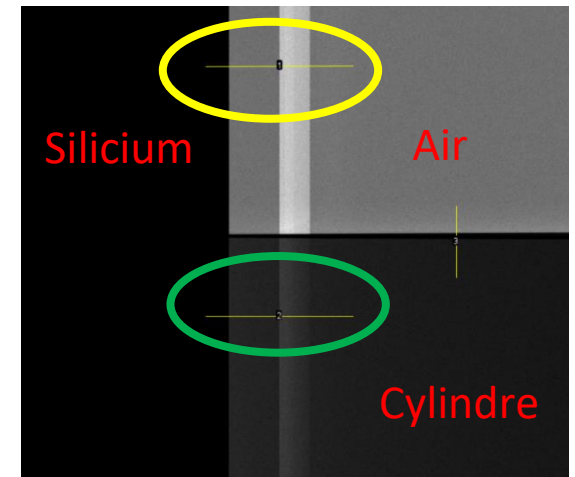


- **GATE (reference)** : refraction profile with **an overshoot**
- **CIVA MC refraction** : **good overall agreement** with GATE in the overshoot region (similar position and amplitude)
- **CIVA Fresnel hybrid** : wave effects are partially smoothed → **attenuated overshoot**, therefore refraction contrast is underestimated

Reflection: MC refraction (CIVA) / Hybrid Fresnel (CIVA) / MC refraction (GATE)



- **GATE** : the presence of the silicon edge introduces **interface effects (reflection)**, visible as over-intensity
- **CIVA MC refraction** : gives a similar profile to GATE, with close intensity levels and a similar decrease
- **CIVA Fresnel hybride** : the model is focused on Fresnel propagation and does not include reflection



Relative errors

Mean relative errors — reference: MC refraction GATE

➤ Refraction :

- MC refraction CIVA vs GATE : **6.52 %**
- CIVA Fresnel hybrid vs GATE : **30.73%**

➤ Reflection 1 :

- CIVA MC refraction vs GATE : **9.63 %**
- CIVA Fresnel hybrid vs GATE : **43.63 %**

➤ Reflection 2 :

- CIVA MC refraction vs GATE : **11.27 %**
- CIVA Fresnel hybrid vs GATE : **39.37 %**

Fresnel hybride :

fast

less accurate on the overshoot and does not model reflection

MC refraction (CIVA) :

best trade-off between **computation time** — around a few minutes — and **profile representativeness**, including both refraction and reflection, close to the GATE reference

Summary and Motivation

➤ CIVA MC refraction :

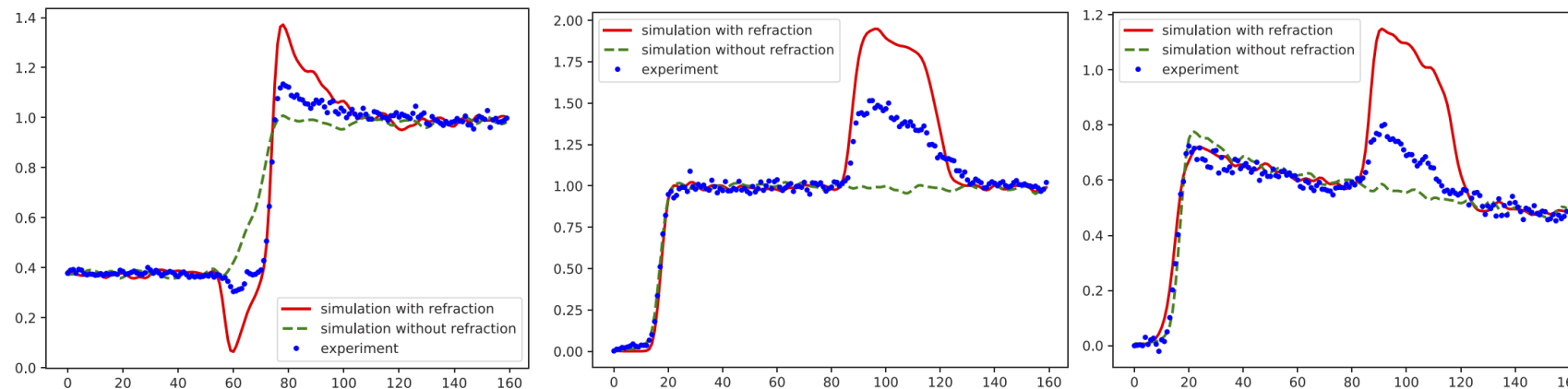
- ☑ good representativeness of the profiles, including refraction and reflection, consistent with the reference

➤ CIVA Fresnel hybrid :

- ☑ simplified and fast model
- ✗ attenuated overshoot, due to smoothed wave effects, and reflection not modeled

➡ MC refraction appears to be the best trade-off between representativeness and computation time; the hybrid model remains a fast approximation.

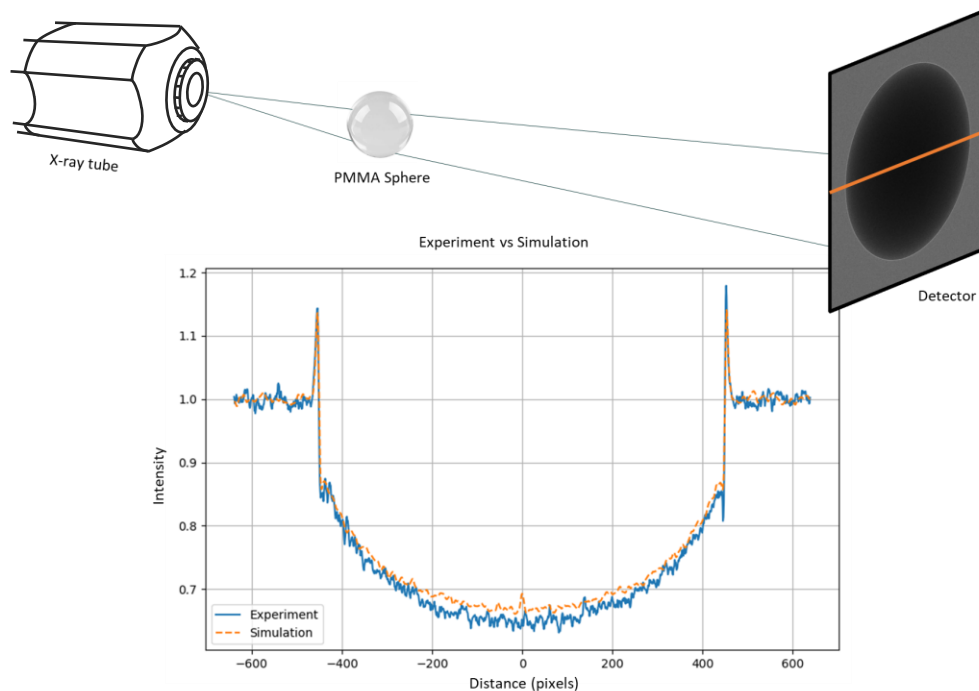
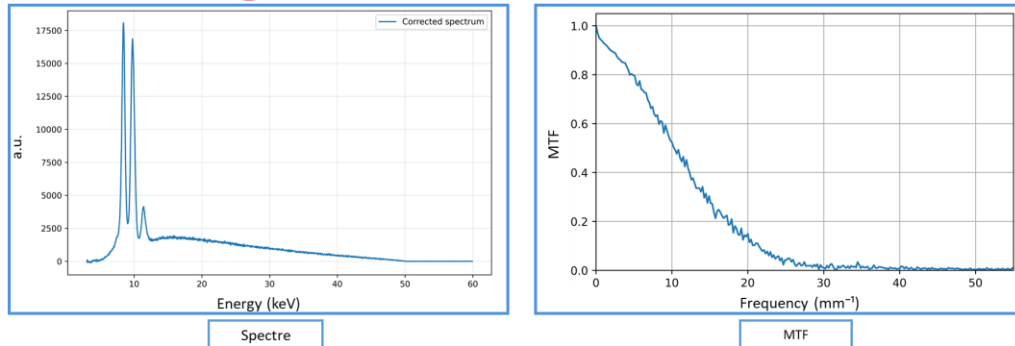
➤ **Intensity-scale difference:** as reported by Max Langer, the simulation shows an **intensity overestimation** compared with the experiment; a similar trend is observed here → need for an **experimental reference + a probabilistic treatment** of the interface.





3 ■ **Experimental configuration**

Review of the case study — Reference experimental configuration



Focal spot

- size and shape estimated
- geometrical blur taken into account

Spectrum

- experimentally measured
- high-voltage correction

MTF

- extracted using the inclined **edge method**
- taking into account the **spatial resolution** (the system's ability to reproduce fine details)

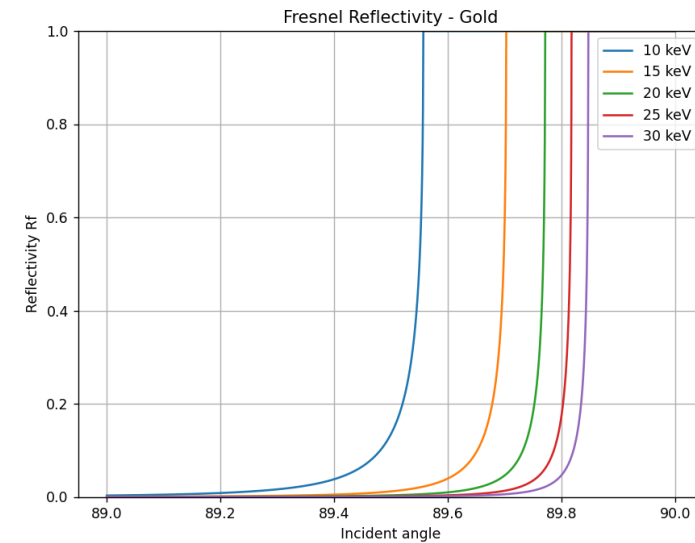


4. Probabilistic model

A probabilistic model at the interface

Reminder — deterministic model

- interface treated using Snell's law
- depending on the angle of incidence:
 - refraction
 - Total reflection



At each interface, the **Fresnel reflectivity** R_f is calculated; it represents the **fraction of reflected energy**

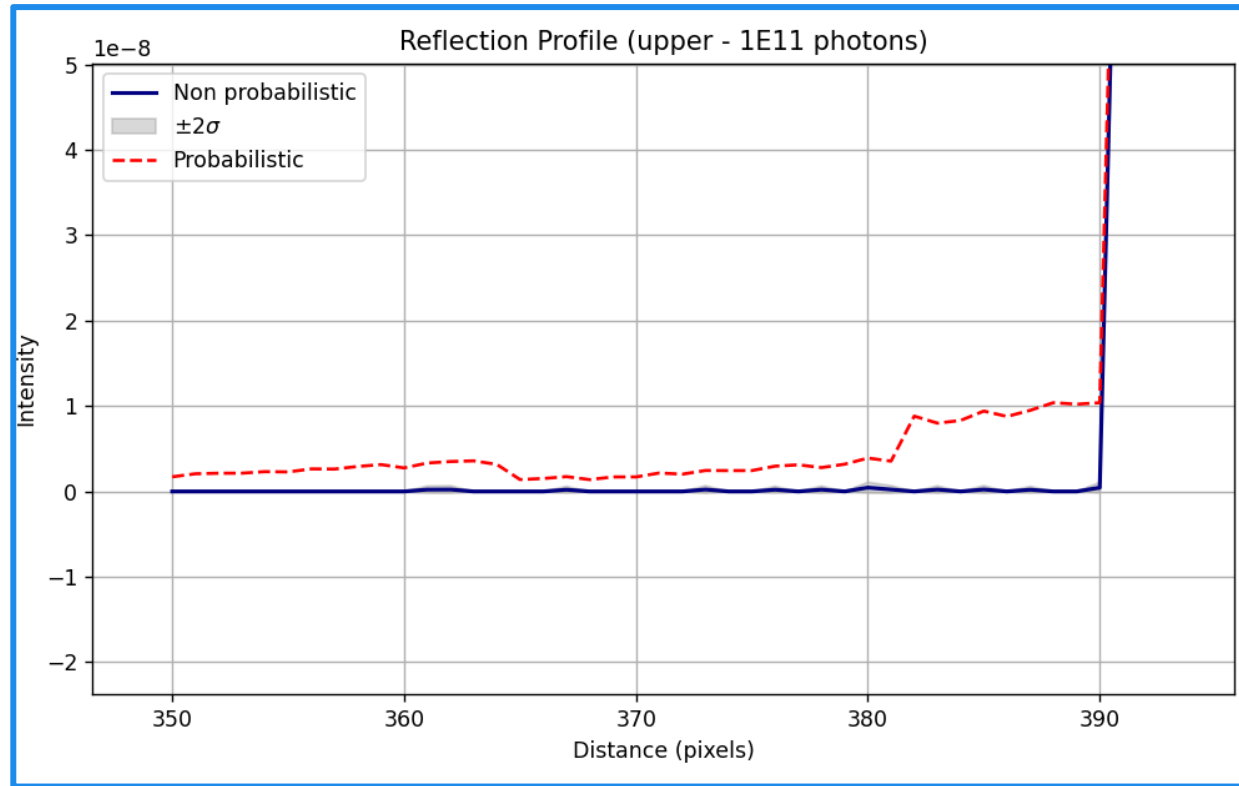
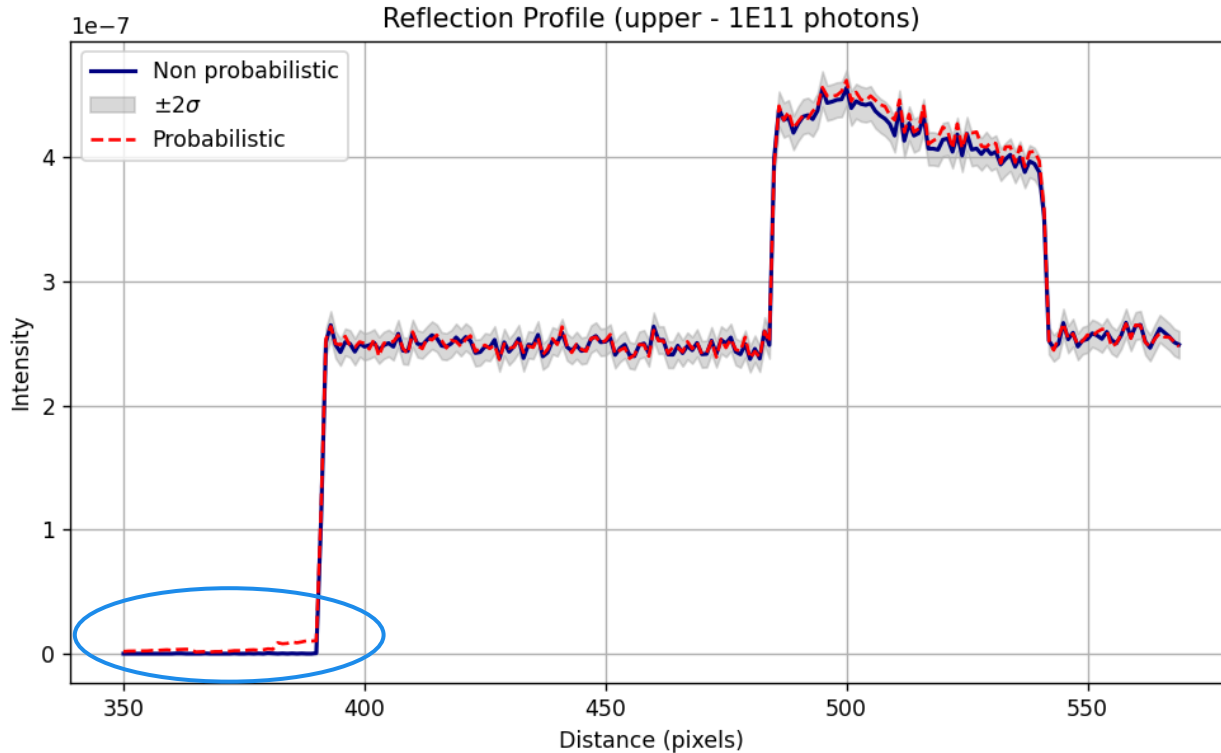
The transmitted / refracted fraction is therefore **$1 - R_f$**

$$w_r = R_f$$

$$w_t = 1 - R_f$$

The incident photon contributes to both branches with different weights

Silicon edge: effect of the probabilistic treatment



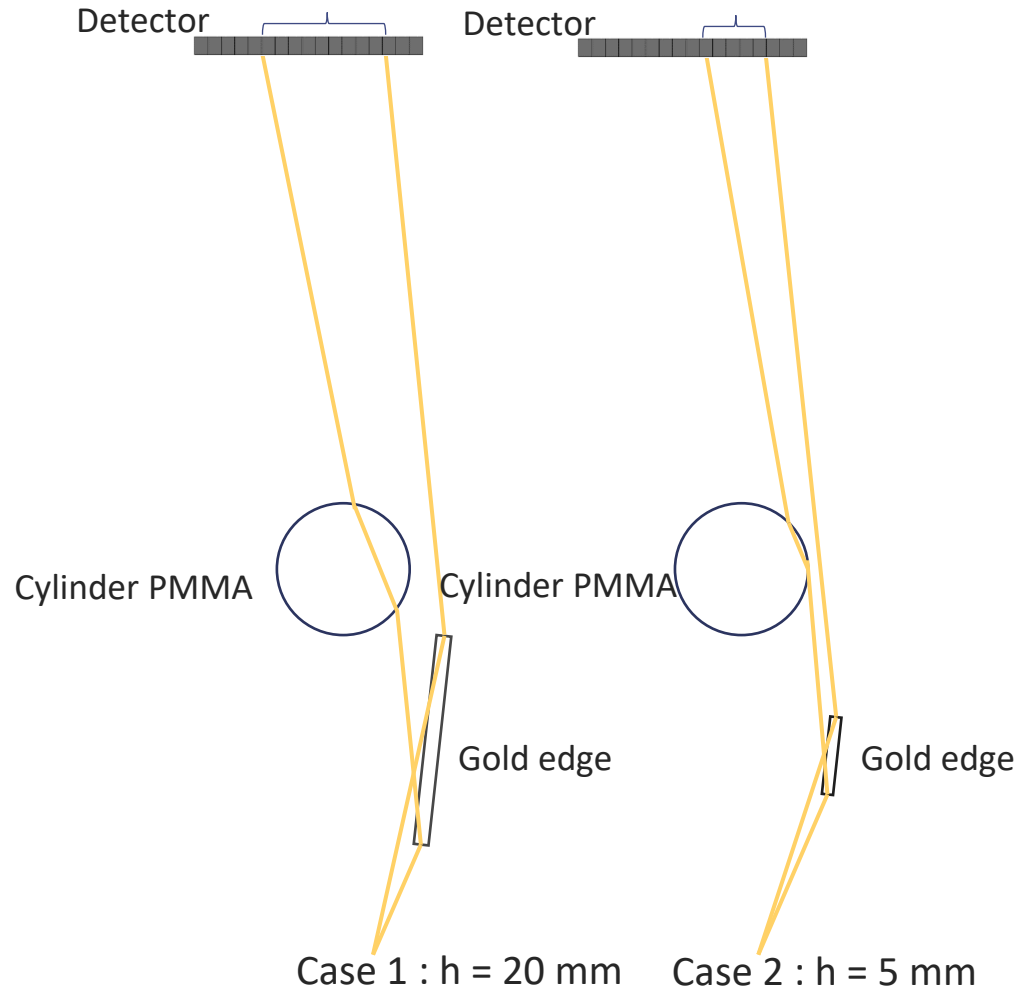
- A small fraction of photons remains refracted in the silicon
- The profiles remain globally similar
- The difference appears mainly near the interface

The probabilistic model highlights this contribution



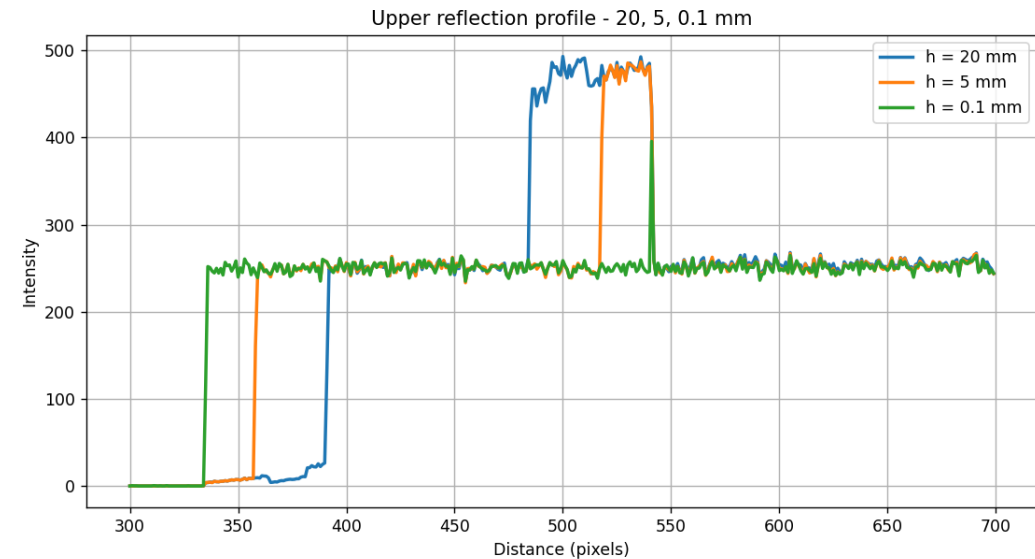
5 ■ Application study

From Max Langer's configuration to gratings: influence of height



Max Langer's configuration can be considered as representative of the elementary components of gratings used in practice.

What happens when the height of this plate is varied?



At the scale of gratings, around $100 \mu\text{m}$, edge refraction becomes difficult to exploit on this profile

Conclusion & Perspectives

Conclusion

- **The MC model** correctly reproduces interface effects in **free-space propagation**
- The **probabilistic treatment** improves the local description **near the interface**
- The parametric study shows that the visibility of the effect strongly depends on the **source, material, and height**
- **Gold is more favorable**, but at the scale of **gratings ($\sim 100 \mu\text{m}$)**, the signature becomes much weaker → **test a configuration with the complete grating**



Perspectives

- **Propagate the output signal** from the object to the detector in order to include **wave effects**
- **Take interference effects into account** in order to access phase information
- Test the model in **grating interferometry**
- Search for a **more favorable configuration** to observe the **probabilistic effect**, with more incident rays at grazing incidence and a sufficient height

Thanks for your attention!

