Modelisation of light transmission through surfaces with optical coating in Geant4

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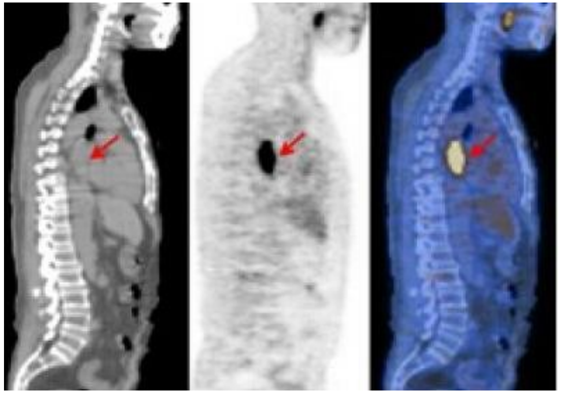
I. Introduction to TOF-PET

PET

- **Functional** imaging technique used in nuclear medecine
- Use **radiotracers** depending on the target (^{18}F-FDG)
- **Gamma rays** detected by scintillator
- Image is reconstructed to form **three-dimensional image**
- **PET/CT** (PET/Scan) overlay of both images



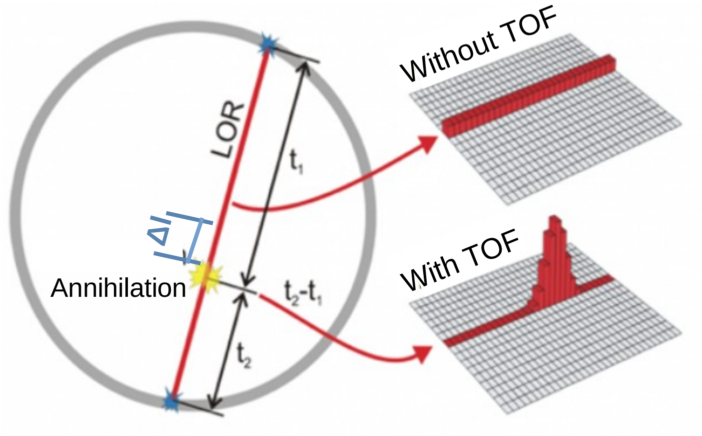
TOF-PET

- Taking care of **the difference between the arrival time** of the two photons on a pair of detectors

$$\boxed{\Delta t = (t_2 - t_1) \pm CTR}$$

$$\boxed{\Delta l = c\frac{\Delta t}{2} \pm c\frac{CTR}{2}} \quad \begin{matrix} CTR = 10\,ps \\ c = 30\,cm.ns^{-1} \end{matrix} \rightarrow \Delta l = c\frac{\Delta t}{2} \pm 1.5\,mm$$

State-of-the-art clinical CTR = 215 ps

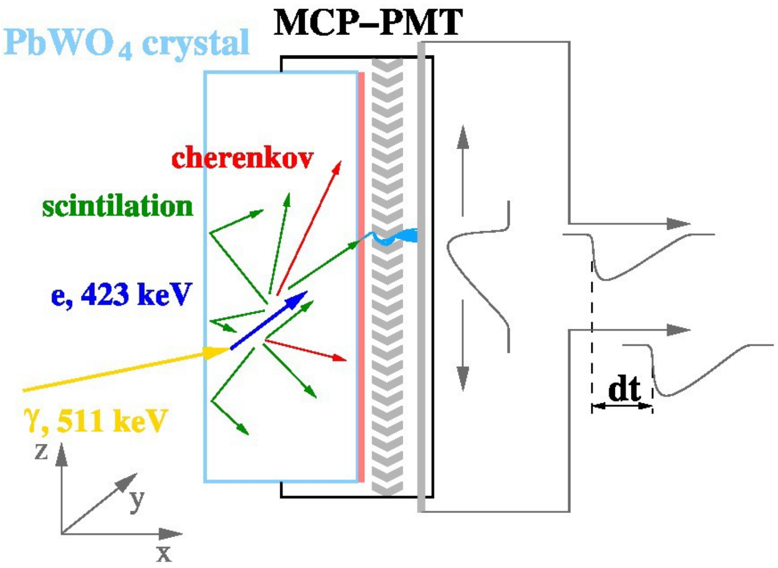


- TOF-PET → improve **SNR** or reduce patient **dose**

II. Goal of the ClearMind project

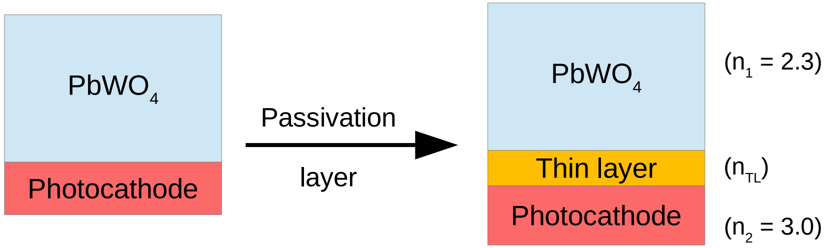
Goal of ClearMind project

- Collaboration between 5 labs
- New PET detector with improved spatio-temporal resolution
  - **$PbWO_4$** crystal: Cerenkov radiator (21 ph/event) and scintillator (200 ph/event), with fast constants (~2 ns)
  - Deposit the photoelectric layer directly on the crystal: **scintronic crystal**
  - Use **Micro-Channel Plate (MCP)**
  - Measure DOI



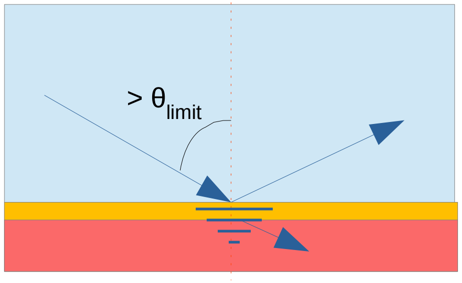
III. Analytical simulation of the impact of the thin layer on a visible photon transmission

Passivation layer introduction



Oxidation of the photocathode by the lead tungstate → **Thin passivation layer** needed

Anti-reflective coating



If $n_1 > n_2$:

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

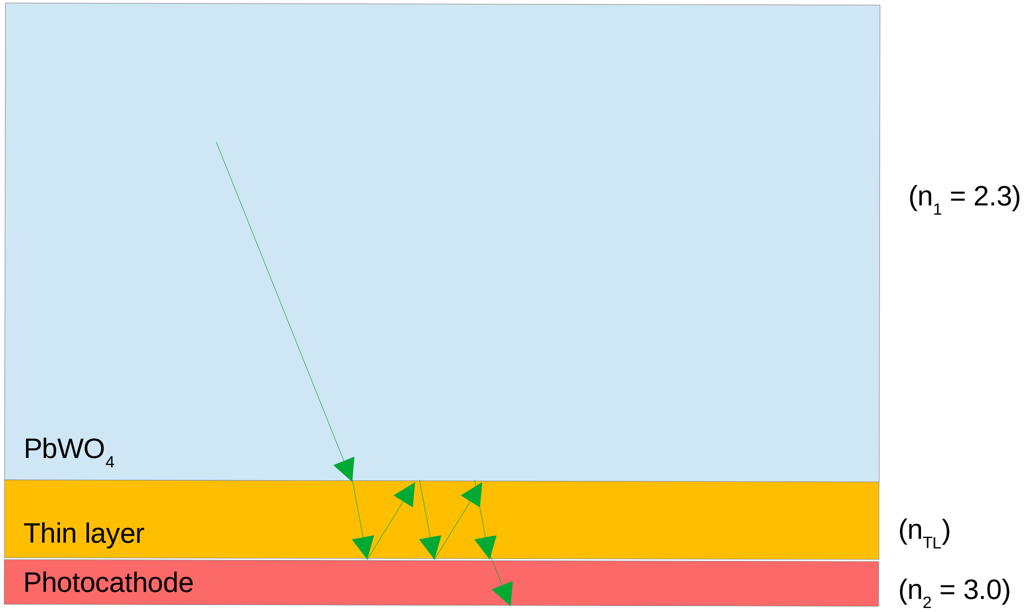
Generates:

- Interference phenomenon at the interfaces
- For $\theta > \theta_{limit}$ an evanescent wave is produced and allows **frustrated transmission**

Iridescence phenomenon

Near field microscopy

Passivation layer introduction



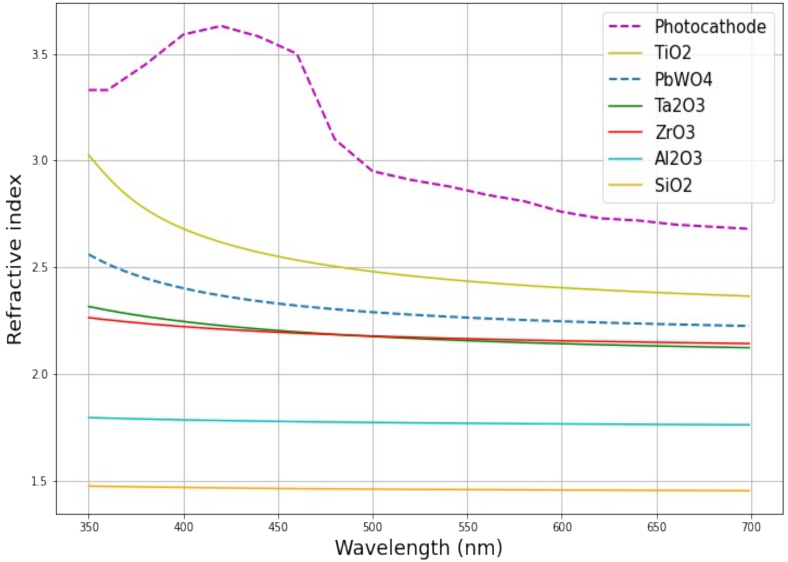
Formulas of reflection and transmission through a thin layer

			Reflection	Transmission		R and T
Simple Interface	Normal incidence		$r_{ij,TE}=r_{ij,TM}=\frac{n_i-n_j}{n_i+n_j}$	$t_{ij,TE}=t_{ij,TM}=\frac{2n_i}{n_i+n_j}$	Fresnel coefficients	$R=\lvert r\rvert^2$
	Oblique incidence	$\theta_1<\theta_{limit}$	$r_{ij,TE}=\frac{n_i\cos\theta_i-n_j\cos\theta_j}{n_i\cos\theta_i+n_j\cos\theta_j}$ $r_{ij,TM}=\frac{n_i\cos\theta_j-n_j\cos\theta_i}{n_i\cos\theta_j+n_j\cos\theta_i}$	$t_{ij,TE}=\frac{2n_i\cos\theta_i}{n_i\cos\theta_i+n_j\cos\theta_j}$ $t_{ij,TM}=\frac{2n_i\cos\theta_i}{n_i\cos\theta_j+n_j\cos\theta_i}$	$r_{TE}+1=t_{TE}$ $n_1(1-r_{TM})=n_2t_{TM}$	$T_I=\frac{n_{end}}{n_{beg}}\lvert t\rvert^2$
		$\theta_1>\theta_{limit}$	Total reflection			
Thin layer	Normal incidence		$r=\frac{r_{12}+r_{23}.e^{2i\beta}}{1+r_{12}.r_{23}.e^{2i\beta}}$	$t=\frac{t_{12}t_{23}e^{i(k_2-k_3)d}}{1+r_{12}r_{23}e^{2i\beta}}\approx\frac{t_{12}t_{23}e^{i\beta}}{1+r_{12}r_{23}e^{2i\beta}}$	$\beta=k_2d$ $k_2=\frac{2\pi}{\lambda_2}=n_2\frac{2\pi}{\lambda_0}=\frac{n_2}{n_1}\frac{2\pi}{\lambda_1}$	$R+T_I\neq1$
	Oblique incidence	$\theta_1<\theta_{limit}$	$r=\frac{r_{12}+r_{23}.e^{2i\beta}}{1+r_{12}.r_{23}.e^{2i\beta}}$	$t=\frac{t_{12}t_{23}e^{i\beta}}{1+r_{12}r_{23}e^{2i\beta}}$	$\beta=k_2d\cos\theta_2$	$T_P=\frac{n_e\cos\theta_e}{n_b\cos\theta_b}\lvert t\rvert^2$
		$\theta_1>\theta_{limit}$	$r=\frac{r_{12}+r_{23}.e^{2\beta}}{1+r_{12}.r_{23}.e^{2\beta}}$	$t=\frac{t_{12}t_{23}e^{\beta}}{1+r_{12}r_{23}e^{2\beta}}$	$\beta=-k_0d\gamma$ $k_0=\frac{2\pi}{\lambda_0}$ $\gamma=\sqrt{n_1^2\sin\theta_1^2-n_2^2}$	
			⚠ Taking r_{ij} for simple interface et $\theta<\theta_{limit}$ replacing $n_2\cos(\theta_2)$ by $i\gamma$ $r_{12,TE}=\frac{n_1\cos\theta_1-i\gamma}{n_1\cos\theta_1+i\gamma}$ $r_{12,TM}=\frac{n_1i\gamma-n_2^2\cos\theta_1}{n_1i\gamma+n_2^2\cos\theta_1}$	$t_{12,TE}=\frac{2n_1\cos\theta_1}{n_1\cos\theta_1+i\gamma}$ $t_{12,TM}=\frac{2n_1n_2\cos\theta_1}{n_1i\gamma+n_2^2\cos\theta_1}$		$R+T_P=1$

M. Born and E. Wolf, Principles of Optics : Electromagnetic Theory of Propagation, Interference and Diffraction of Light, ch. Basic properties of electromagnetic field. Elsevier, June 2013.

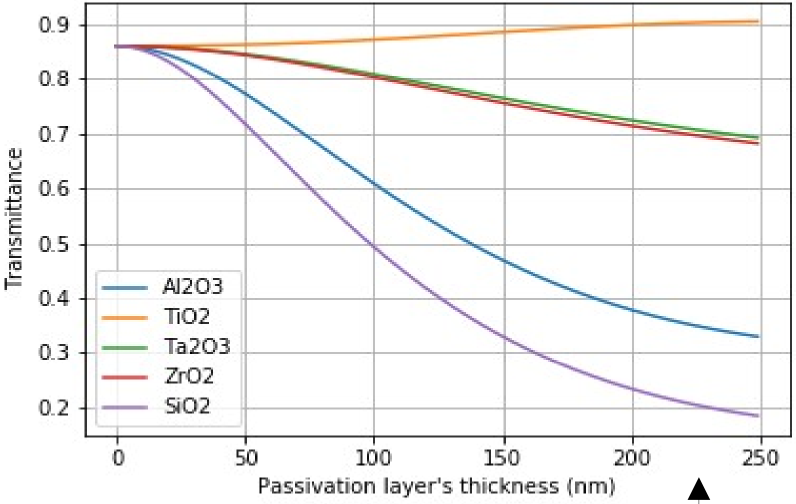
Comparison of passivation layer materials

- Comparison of:
  - Zirconium oxide, ZrO_3
  - Tantalum oxide, Ta_2O_3
  - Aluminium oxide, Al_2O_3
  - Titanium oxide, TiO_2
  - Silicon oxide/Quartz, SiO_2
- No frustrated transmission with TiO_2

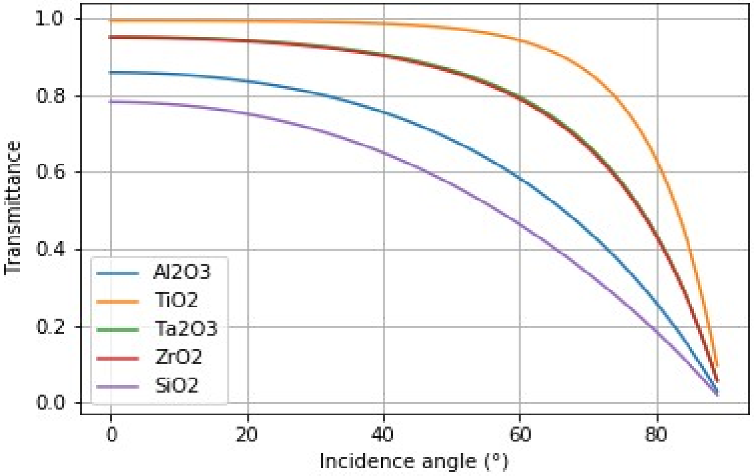


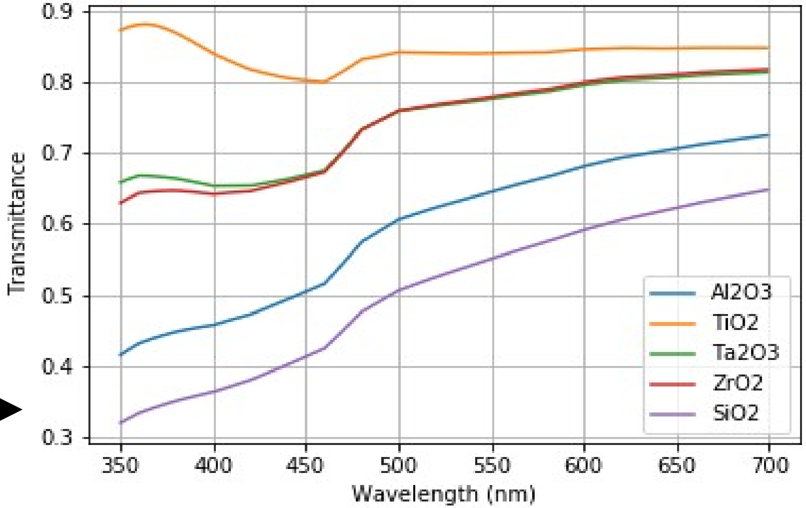
Refractive index as a function of the wavelength

Comparison of passivation layer materials



Transmittance as a function of incidence angle and integrated over PWO emission spectrum for a 100 nm-thick passivation layer





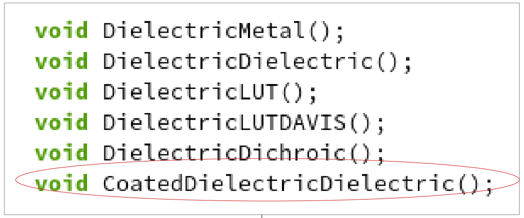
Transmittance as a function of layer thickness and integrated over PWO emission spectrum and incidence angles

Transmittance as a function of wavelength integrated over incidence angles for a 100 nm-thick passivation layer

IV. Implementation of interferences and frustrated transmission in Geant4

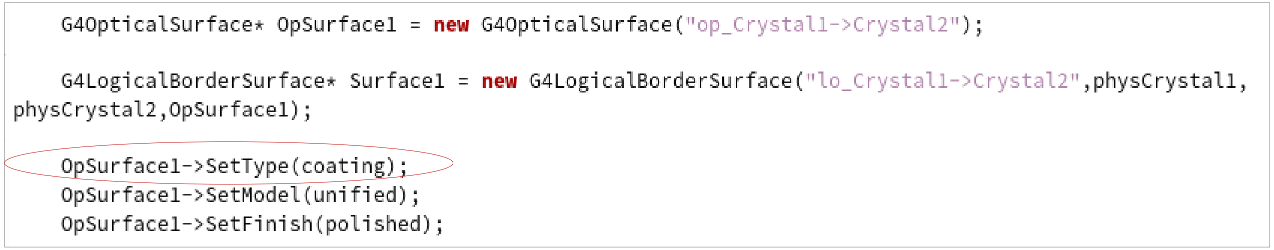
Integration of interferences and frustrated transmission due to a thin layer in Geant4

G4OpBoundaryProcess.h

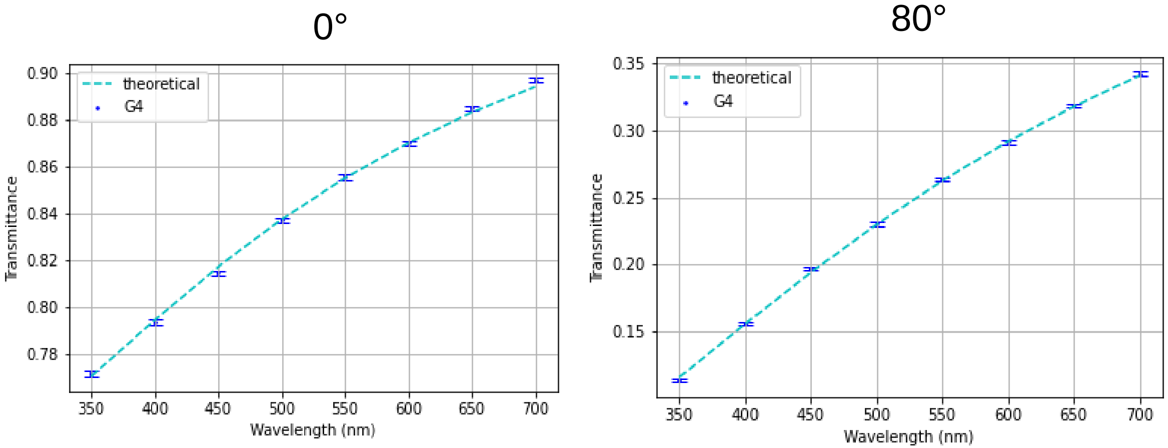


```
void DielectricMetal();
void DielectricDielectric();
void DielectricLUT();
void DielectricLUTDAVIS();
void DielectricDichroic();
void CoatedDielectricDielectric();
```

DetectorConstruction.cc



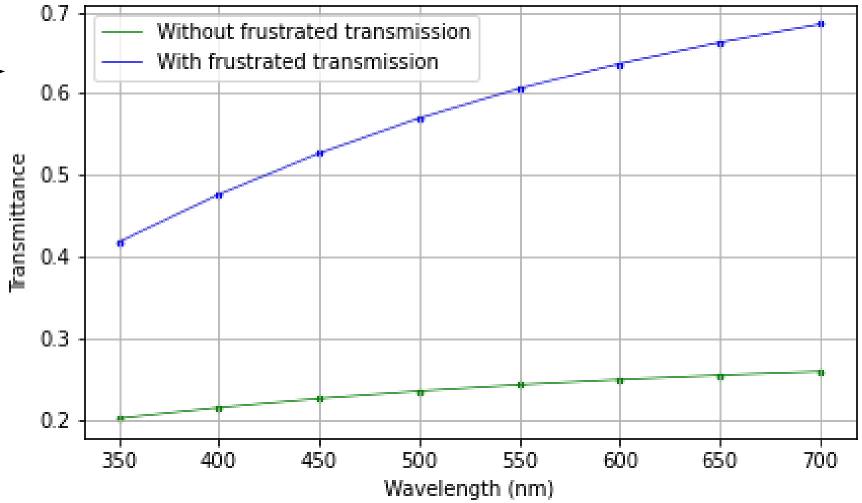
```
    G4OpticalSurface* OpSurface1 = new G4OpticalSurface("op_Crystal1->Crystal2");

    G4LogicalBorderSurface* Surface1 = new G4LogicalBorderSurface("lo_Crystal1->Crystal2",physCrystal1,
physCrystal2,OpSurface1);

    OpSurface1->SetType(coating);
    OpSurface1->SetModel(unified);
    OpSurface1->SetFinish(polished);
```



Example of transmittance for a visible photon passing through a thin layer of 100 nm SiO_2 as a function of wavelength for two incidence angles

What is the importance of frustrated transmission through a thin layer?

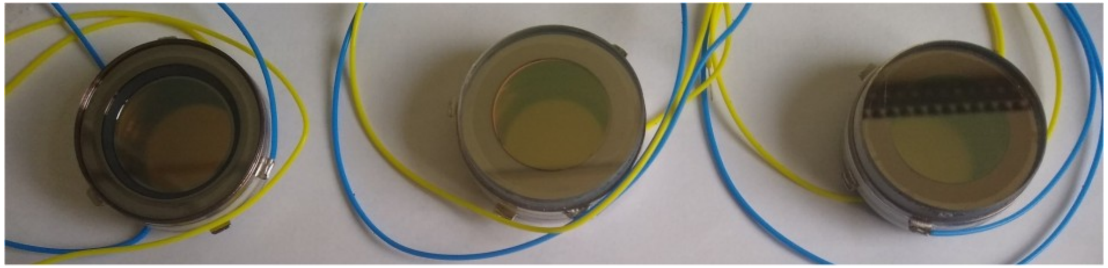
Transmittance through a thin layer as a function of wavelength integrated over incidence angles, with and without frustrated transmission



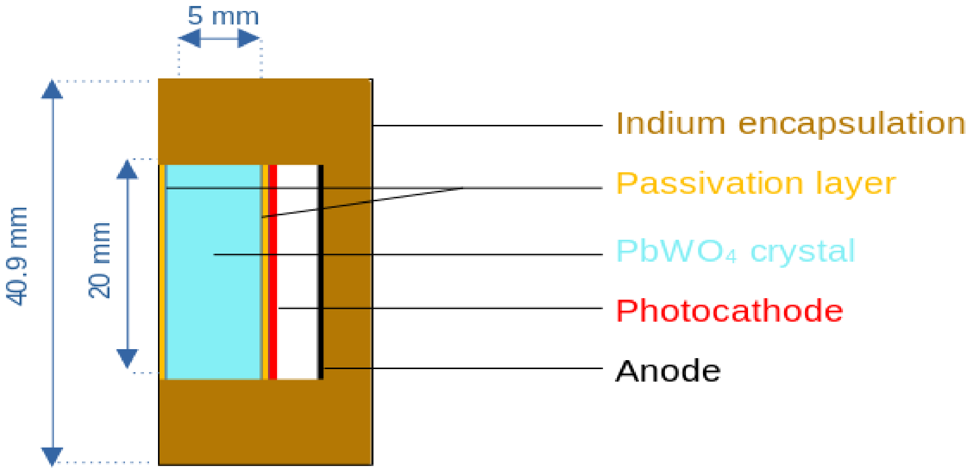
- Simulation of transmittance through thin layer with frustrated transmission for large angles (blue curve) and with total reflection only for large angles (green curve)
- The transmittance is **two times increased** thanks to frustrated transmission

V. Experimental studies on Photek test cells

Experimental studies on Photek test cells

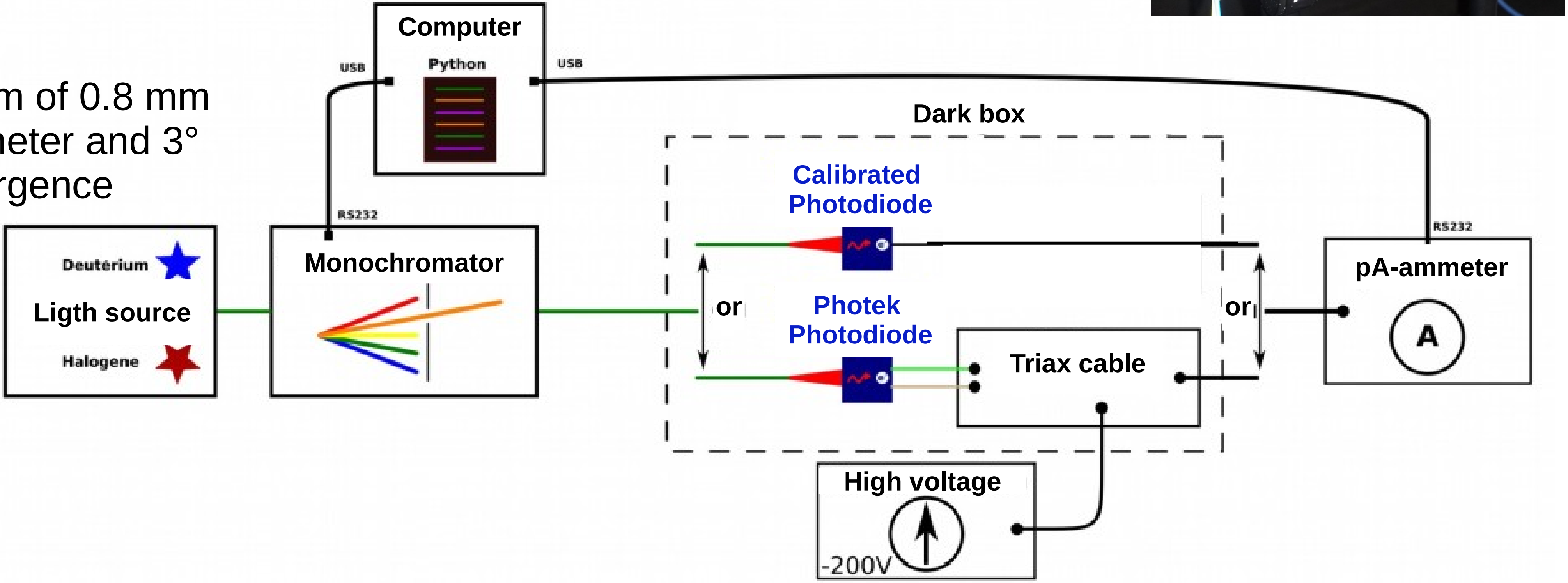


- Photek test cells:
  - SiO_2, without thin layer
  - $PbWO_4$ 2018
  - $PbWO_4$ 2021



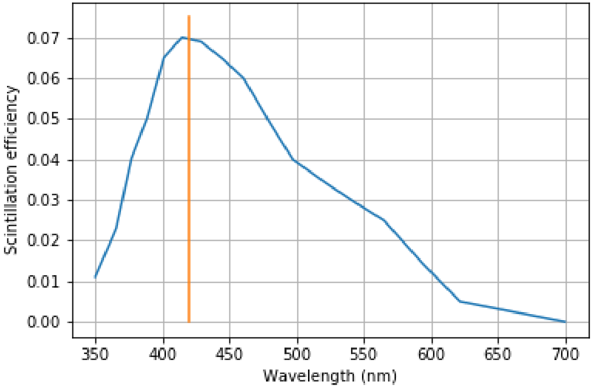
Measurement setup

Beam of 0.8 mm diameter and 3° divergence

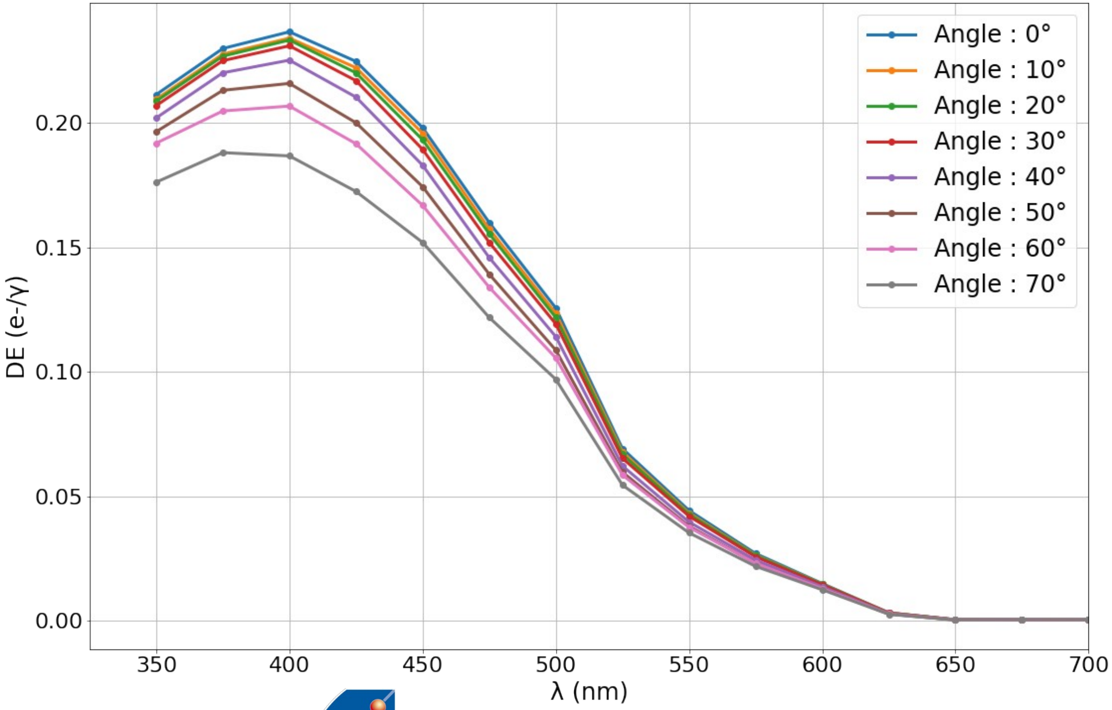


Analysis of experimental data

Emission spectrum of lead tungstate



Detection Efficiency (DE) of Photek PWO2018 as a function of wavelength (λ)



$$DE \equiv QE \times Transmittance$$

$$DE = \frac{S_{PHOTEK}\, h\, c}{e\, \lambda}$$

S_{PHOTEK} : Sensitivity of Photek test cells [A/W]

$$S_{PHOTEK} = \frac{I_{PHOTEK}\, S_{CAL}}{I_{CAL}}$$

Work in progress...

Conclusion and perspectives

- The **theoretical description** of the passivation layer shows an impact on the transmittance of visible photons
- This theoretical model has been integrated in **Geant4** to describe an interface containing a thin layer
- **Measurements are carried on at CEA-Saclay** for assessment

Thank you for your attention