Modelisation of light transmission through surfaces with optical coating in Geant4

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I. Introduction of TOF-PET

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TOF-PET

- Taking care of **the difference between the arrival time** of the two photons
- Estimating annihilation position
- Needing fast detectors
- Improving **SNR** or reducing the patient **dose**
- **10 ps challenge**

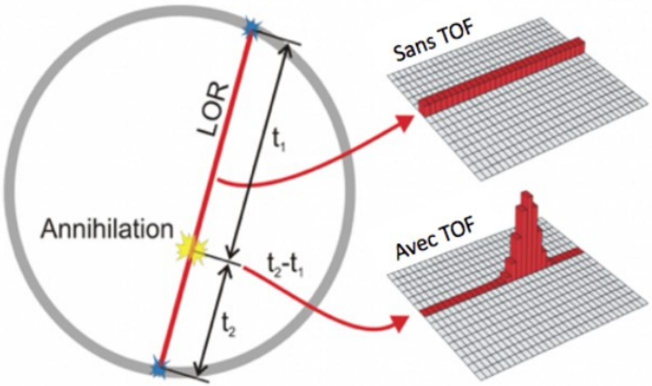
$$\Delta t = (t_2 - t_1) \pm CTR$$

$$\Delta l = c\frac{\Delta t}{2} \pm c\frac{CTR}{2}$$

$c = 30\, cm.ns^{-1}$

if $CTR = 10\, ps$

then $\rightarrow \Delta l = 1{,}5\, mm$



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II. Goal of ClearMind project

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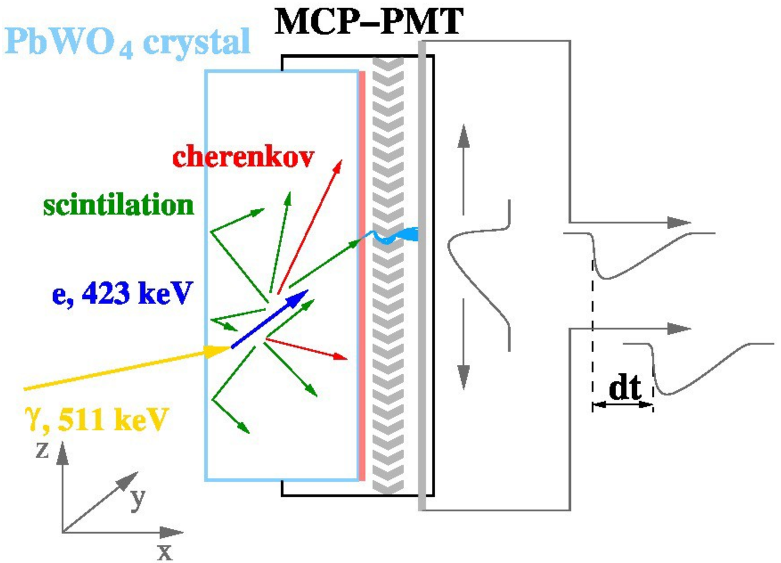
Goal of ClearMind project

- Collaboration between CEA-IRFU, IJCLab and CPPM
- New PET detector with improved spatio-temporal resolution
  - **$PbWO_4$** crystal: Cerenkov (21 photon/event) and scintillation (200 photon/event) production, with fast constants (~2 ns)
  - Deposit the photoelectric layer directly on the crystal : **scintronic crystal**
  - Use **MicroChannel Plate (MCP)**
  - Measure DOI



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

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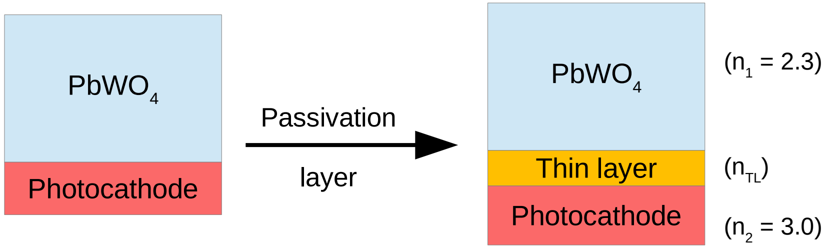
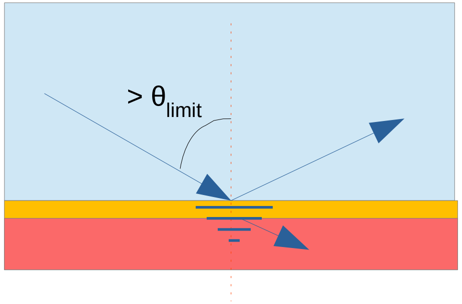
Passivation layer introduction





If $n_1 > n_2$:

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

- Lead tungstate alters the photocathode → **Thin passivation layer needed**

- Generates interference phenomenon at the interfaces

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

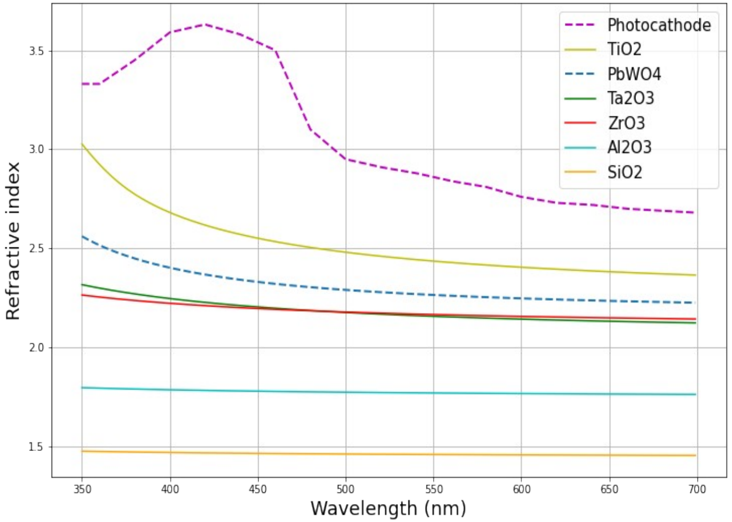
Formulas of reflection and transmission through a thin layer

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

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



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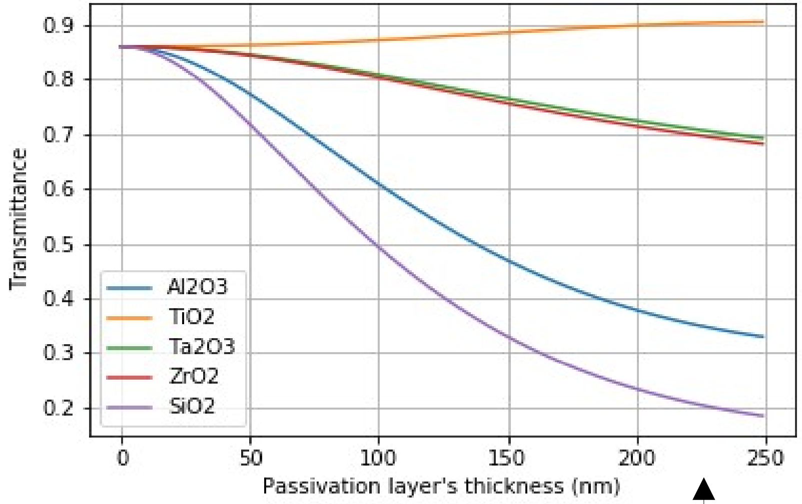
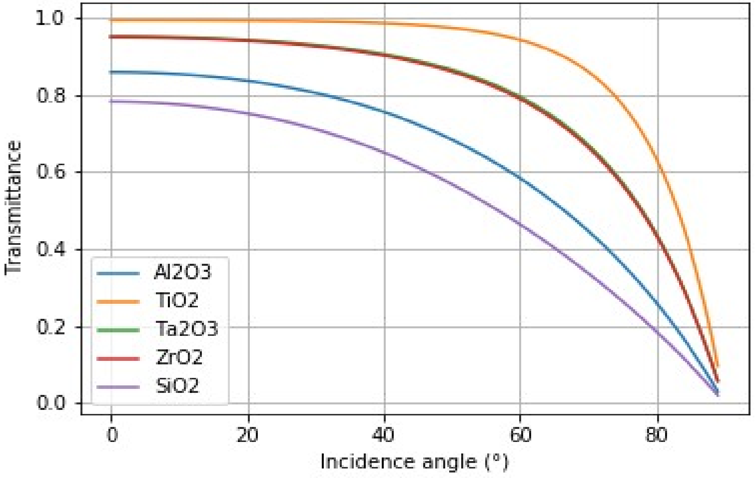
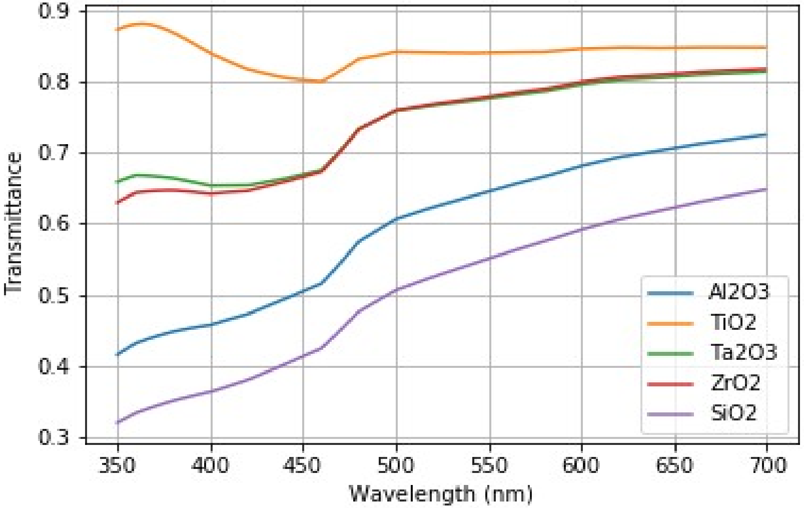
Comparison of passivation layer materials



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



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



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

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IV. Implementation of interferences and frustrated transmission in Geant4

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

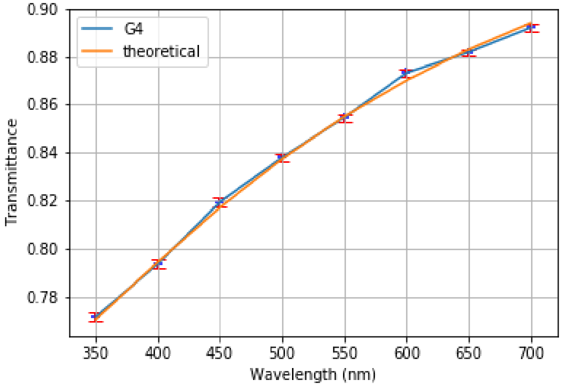
G4OpBoundaryProcess.h

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

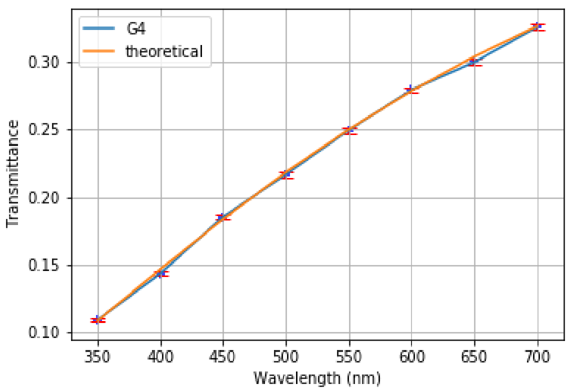
DetectorConstruction.cc

```
    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);
```

0°



80°



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

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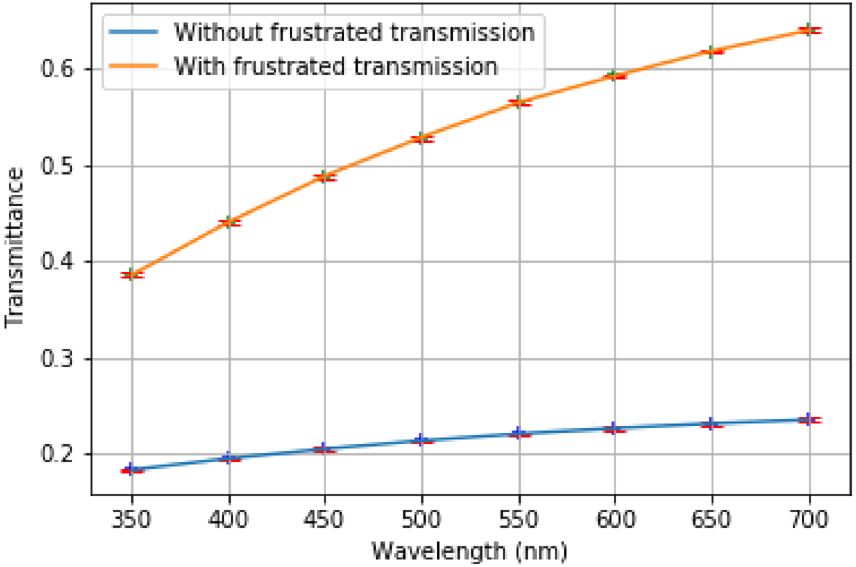
What is the importance of frustrated transmission through a the thin layer?

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 (orange curve) and with total reflection for large angles (blue curve)
- The transmittance is **two time increased** thanks to frustrated transmission

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V. Experimental studies on Photek test cells

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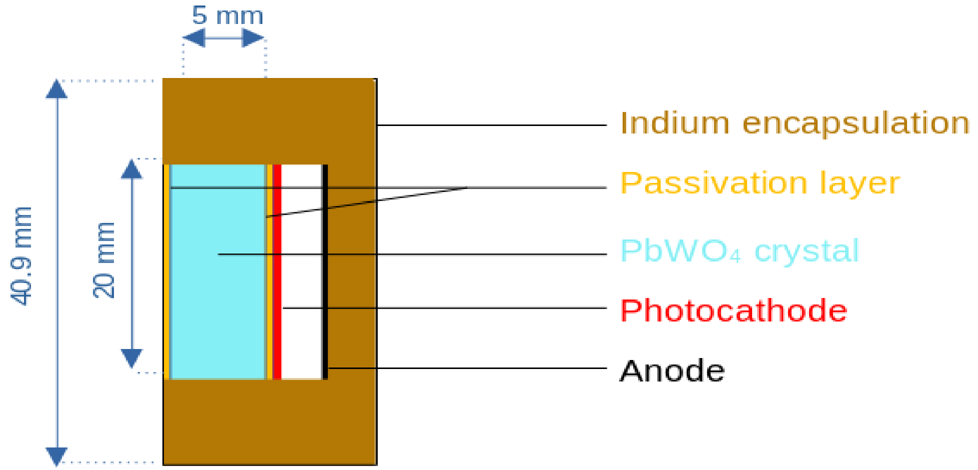
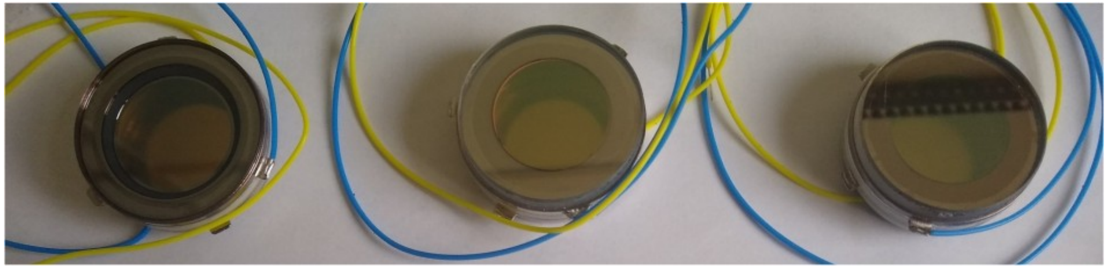
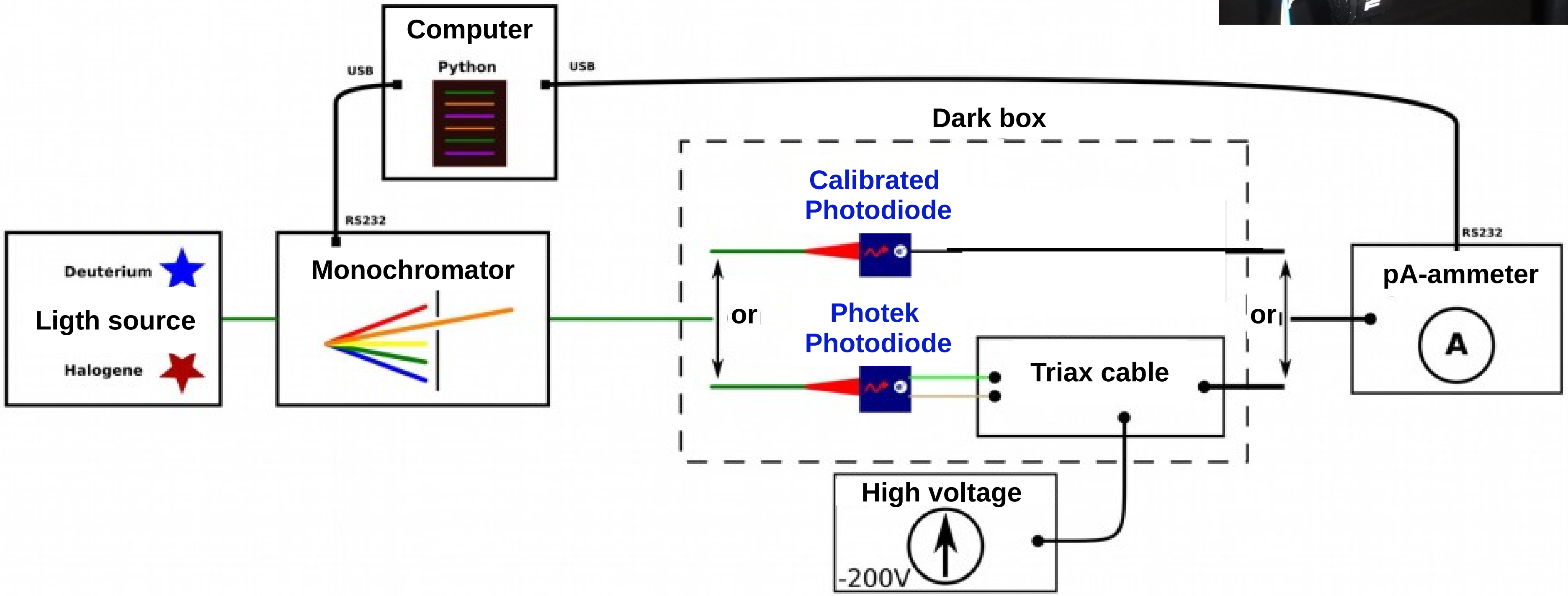
Experimental studies on Photek test cells

- Photek test cells:
  - SiO_2, without thin layer
  - $PbWO_4$ 2018
  - $PbWO_4$ 2021
- Beam of 0.8 mm diameter and 3° maximum divergence





Measurement setup



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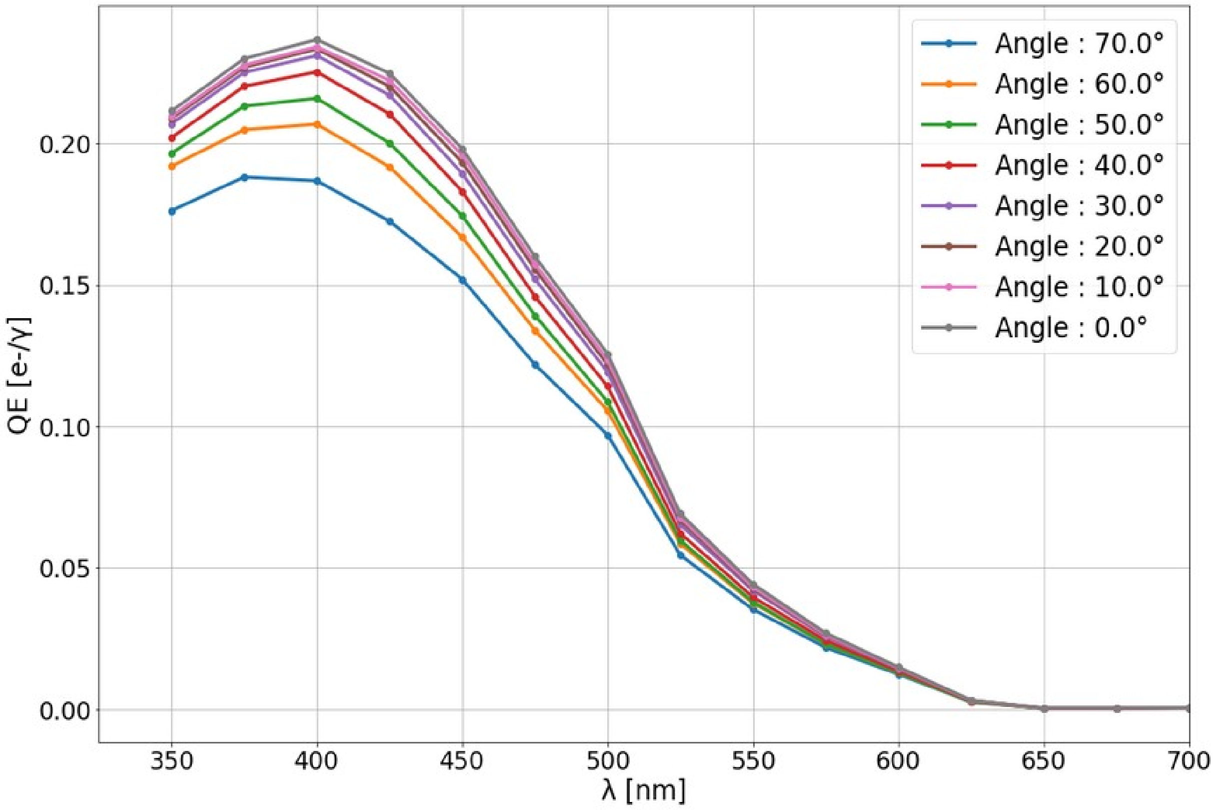
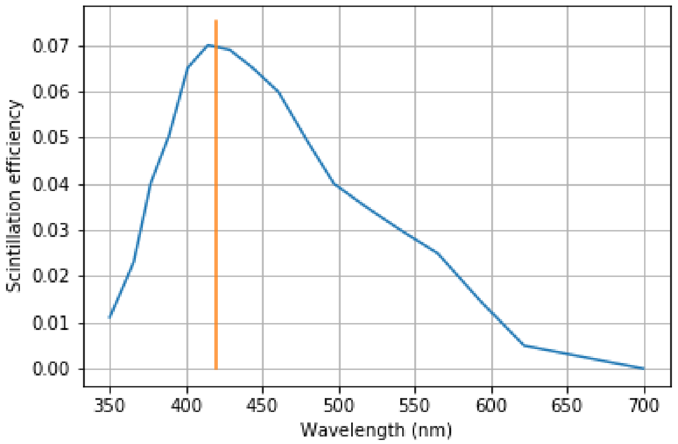
Quantum efficiency of Photek photocathode as function of wavelength





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

$$QE = \frac{S_{PH} h c}{q \lambda}$$

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Conclusion and perspectives

- The **theoretical description** of the passivation layer shows an impact on the transmittance of visible photons
- This theretical model as been intergrated in **Geant4** to describe an interface composed with thin layer
- **Measurement are carried on at CEA-Saclay** for assessement

Thank you for your attention

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