Update of the optical light transport in Geant4 to model optical coating

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I. Context: the ClearMind project

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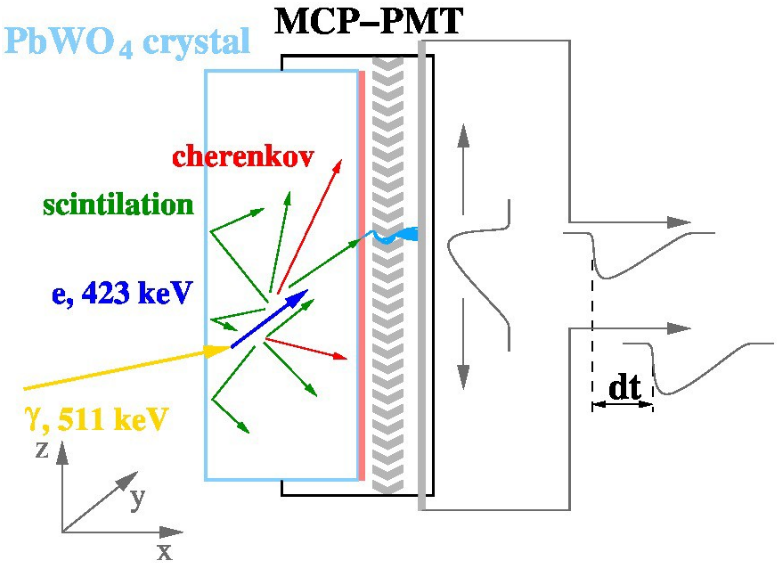
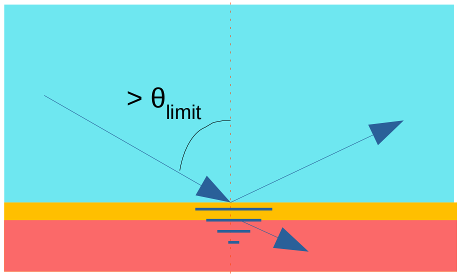
Introduction of the ClearMind project

- Collaboration between CEA-IRFU, IJCLab and CPPM
- New PET detector with improved spatio-temporal resolution
  - **PWO** crystal: Cerenkov (21 photon/event at 511 keV) and scintillation (200 photon/event at 511 keV) production, with fast constants (~2 ns)
  - Deposit the photoelectric layer ($n_{PC} > n_{PWO}$) directly on the crystal: **scintronic crystal** to improve detection efficiency
  - Use **Micro-Channel Plate (MCP-PMT)** for precise timing
  - **Passivation** of PWO/PC interface to protect photocathode from oxidation



Thin layer introduction

Anti-reflective coating



If $n_1 > n_{TL}$:

$$\theta_L = \arcsin\left(\frac{n_{TL}}{n_1}\right)$$

Consequences

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

Iridescence phenomenon

Near field microscopy

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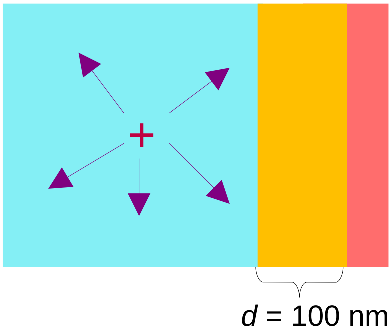
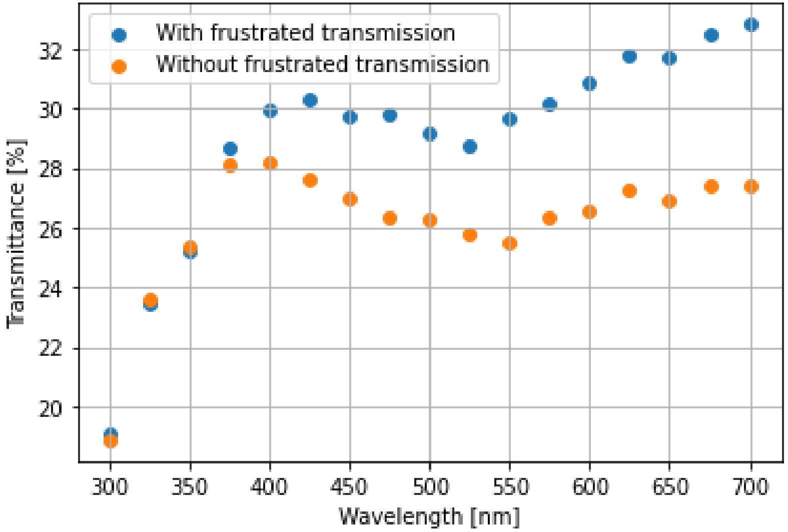
Importance of the frustrated transmission



- Three medium PWO, TL, PC
- TL: thin layer with 100 nm thickness
- Absorption length of the crystal is fixed
- Optical photons generated from the center of the cristal
- Isotropically

Transmittance to photocathode with and without frustrated transmission as a function of wavelength for isotropic photon generation



→ Transmittance **increases by 4 %** thanks to **frustrated transmission**

→ **Simulation of thin layer phenomena is essentials**

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II. Implementation in Geant4

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Integration of thin layer in Geant4

- New function in G4OpBoundaryProcess class,

based on DielectricDielectric()

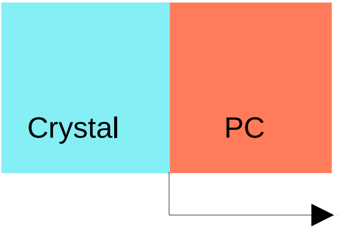
```
void DielectricMetal();
void DielectricDielectric();
void DielectricLUT();
void DielectricLUTDAVIS();
void DielectricDichroic();
void CoatedDielectricDielectric();
```

- New Surface Type:

```
enum G4SurfaceType
{
   dielectric_metal,
   dielectric_dielectric,
   coated,
   dielectric_LUT,
   dielectric_LUTDAVIS,
   dielectric_dichroic,
   firsov,
   x_ray
};
```

- New Status:

```
enum G4OpBoundaryProcessStatus
{
  Undefined,
  Transmission,
  FresnelRefraction,
  FresnelReflection,
  TotalInternalReflection,
  LambertianReflection,
.
.
.
  Dichroic,
  CoatedDielectricReflection,
  CoatedDielectricRefraction,
  CoatedDielectricFrustratedTransmission
};
```



- thickness ? → Thickness*TL*
- refractive index ? → *RindexTL*
- *frustrated ?*

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III. Theoretical transmittance through the thin layer

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Formulas of reflection and transmission

Fresnel coefficient (used by DielectricDielectric())

		Reflection	Transmission
Normal incidence		$r_{ij,TE}=r_{ij,TM}=\frac{n_i-n_j}{n_i+n_j}$	$t_{ij,TE}=t_{ij,TM}=\frac{2n_i}{n_i+n_j}$
Oblique incidence	$\theta_i < \theta_l$	$r_{ij,TE}=\frac{n_i\cos\theta_i-n_j\cos\theta_j}{n_i\cos\theta_i+n_j\cos\theta_j}$ $r_{ij,TM}=\frac{n_i\cos\theta_j-n_j\cos\theta_i}{n_i\cos\theta_j+n_j\cos\theta_i}$	$t_{ij,TE}=\frac{2n_i\cos\theta_i}{n_i\cos\theta_i+n_j\cos\theta_j}$ $t_{ij,TM}=\frac{2n_i\cos\theta_i}{n_i\cos\theta_j+n_j\cos\theta_i}$
	$\theta_i > \theta_l$	Total internal reflection	

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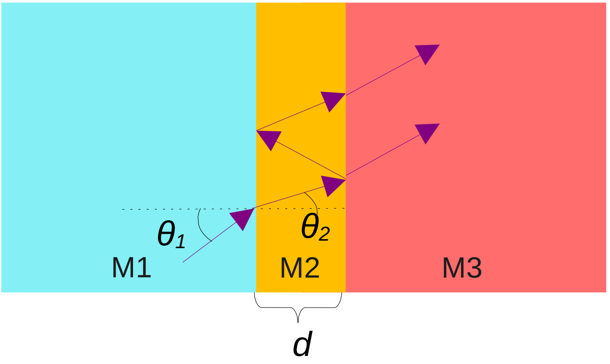
Formulas of reflection and transmission



Coefficient of transmission and reflection through thin layer

(used by CoatedDielectricDielectric())

$\theta_1 < \theta_L$:	$\theta_1 \geq \theta_L$:
θ_2 existed $\beta = k_2 d \cos(\theta_2)$	θ_2 doesn't existed → remplacing $n_2\cos\theta_2$ by $i\gamma$ in Fresnel coefficient $\gamma = \sqrt{n_1^2 \sin(\theta_1)^2 - n_2^2}$ $\beta = ik_0 d\,\gamma$

$$t = \frac{t_{12} t_{23} e^{i\beta}}{1 + r_{12} r_{23} e^{2i\beta}}$$

$$r = \frac{r_{12} + r_{23} . e^{2i\beta}}{1 + r_{12} . r_{23} . e^{2i\beta}}$$

Not possible in Geant4 yet

$$k_2 = n_2 \frac{2\pi}{\lambda} = k_0 x n_2$$

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IV. Comparison between theoretical and simulated transmittances

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Correctness of the implementation

	What we want to simulate	What we code in Geant4
Simple interface	$n_1 = 1.5$ | $n_2 = 1.0$	Physical and Logical Volume: 1 and 2 Optical Surface Types: *dielectric_dielectric* Optical photons generated inside M1
Interface composed with thin layer	$n_1 = 1.5$ | $n_2 = 1.5$ $n_{TL} = 1.0$	Physical and Logical Volume: 1 and 2 Optical Surface Types: *coated* → Thickness and Refractive Index of TL Optical photons generated inside M1

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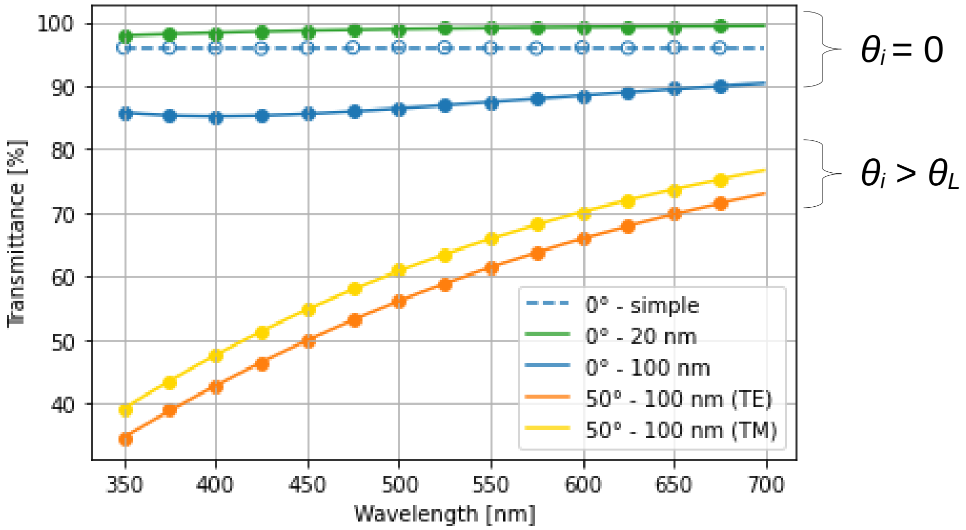
Correctness of the implementation

— Theory
● Simulation

$$Transmittance = \frac{Photons\ inside\ Volume\ 2}{Generated\ photons}$$



Correct implementation of the model in the Geant4 software

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V. Experimental validation of the implemented model

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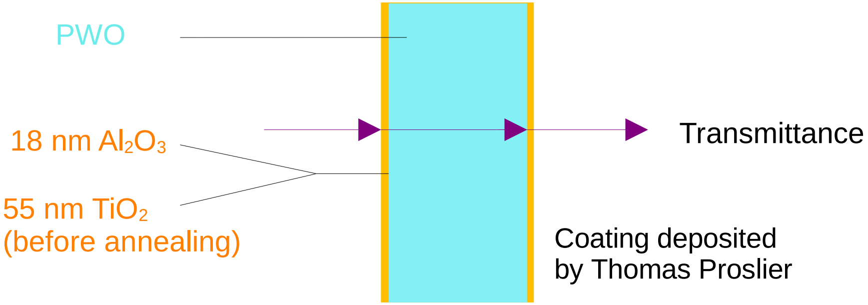
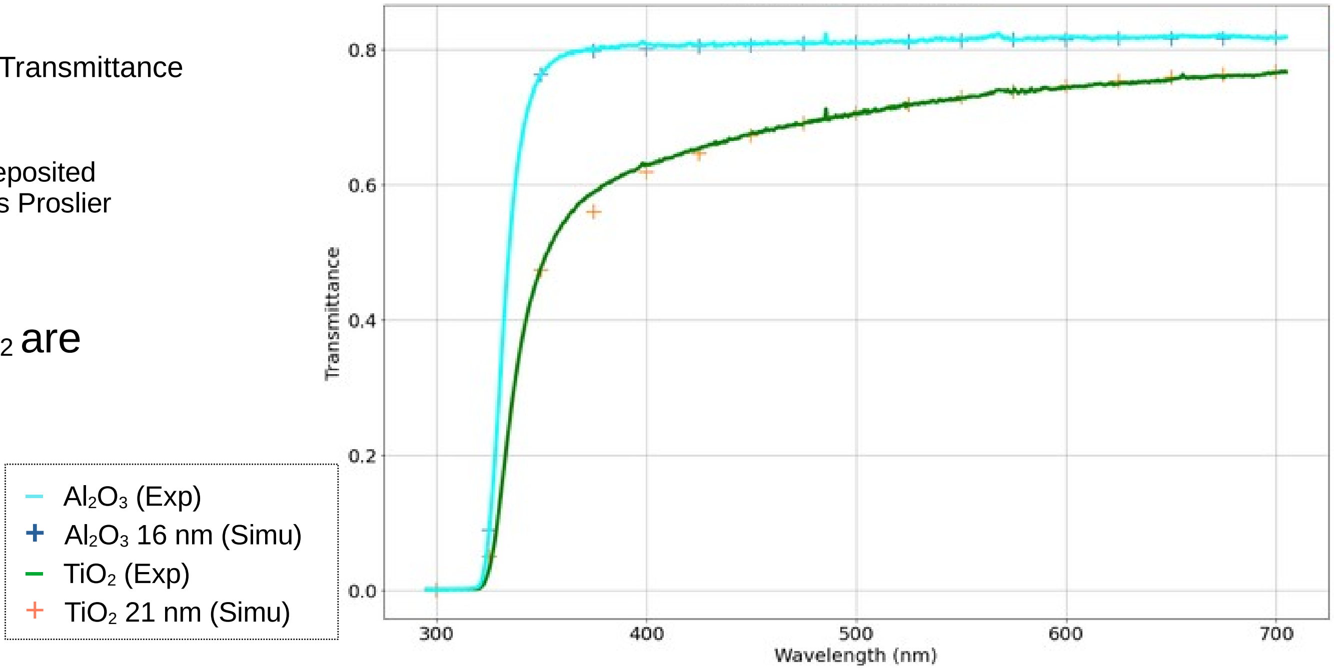
Experimental validation



Hypothesis:
- Refractive index of Al_2O_3 and TiO_2 are known

Unknown variables:
- Thickness of passivation layer
- Refractive index of PWO
- Attenuation length of PWO

Transmittance as function of wavelength, through a window optically coated on both its faces, depending of the thin layer materials



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Conclusion

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- Simulation of transmittance through thin layer with Geant4 is essential to model the ClearMind detector
- Perfect agreement between simulated and theoretical transmittance
- The model has also been validated experimentally
- This update may be of interest for any modeling of light transport including optical coating in G4

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