Geant4 Studies of the scintillator crystals for the axial HPD-PET concept

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Abstract — The 3D Axial HPD-PET concept consists of axially oriented arrays of long and thin scintillator crystal bars read-out at both ends by a Hybrid Photon Detector. In the framework of feasibility studies various investigations are being performed about the characteristics of the crystals to be employed. The resolution in terms of the axial reconstruction of a single gamma ray \( \sigma \) and its energy \( \sigma_{E}/E \) depend on the physical and optical properties of the chosen scintillator, including its surface finish (coating/wrapping), and on the characteristics of the photodetectors. A comparison of computational studies carried out with Geant4 for YAP:Ce crystal bars of dimensions 3.2\times3.2\times100 \text{ mm}^3 and experimental results allows to evaluate the influence of the optical parameters of the crystal lateral surfaces on the light collection. The measurements of the effective light attenuation lengths and of the axial resolutions are well reproduced by the Geant4 results. With the thus validated simulations we show that a mechanical structuring of the crystal surface, which leads to pure surface absorption, would allow to significantly enhance the PET detector performance. This method to adjust the effective absorption length promises good reproducibility in the production of large numbers of crystals.

Index Terms — Geant4; YAP:Ce; molecular imaging; PET.

I. INTRODUCTION

Recently a novel 3D PET geometrical concept has been proposed \cite{1}. It is based on axially oriented arrays of long (10-15 cm) and thin polished scintillator bars read out at the two ends by Hybrid Photodetectors (HPD) \cite{2}. The concept allows for an unambiguous reconstruction in 3D of the photon’s interaction point eliminating the Depth of Interaction (DoI) uncertainty. The axial coordinate \( z \) is obtained from the ratio of the light quantity at the two crystal ends. The 3D Axial HPD-PET concept provides higher detection efficiency due to the absence of limitations imposed by the detector thickness in the radial direction, and to the possibility \cite{1} to recover a fraction of \( \gamma \)’s undergoing double interactions (first Compton and then photoelectric) in the crystal array.

The resolutions of the axial \( z \) coordinate (\( \sigma_z \)), the gamma ray energy (\( \sigma_{E}/E \)), and the detection time (\( \sigma_t \)) of the device are influenced \cite{1,3} by \( \lambda_{\text{eff}} \) and \( N_0 \), the key parameters of the HPD-PET concept. The effective light attenuation length \( \lambda_{\text{eff}} \) describes the absorption of photons along their path inside the crystal from the scintillation point to the photodetectors. \( \lambda_{\text{eff}} \) is about 20\% smaller than the bulk absorption length \( \lambda_{\text{bulk}} \) as it relates to the projected axial path length. \( N_0 \) is the number of photoelectrons (pe’s) detected for a 511 keV \( \gamma \)-ray in a crystal bar without any light absorption (\( \lambda_{\text{eff}} = \infty \)). Its value depends both on the physical and optical properties of the chosen scintillator and of its surface, and on the characteristics of the photodetector. While an increase of \( N_0 \) improves the resolution of all 3 quantities (\( z, E, t \)), a longer \( \lambda_{\text{eff}} \) improves \( \sigma_{E}/E \) and \( \sigma_t \), however it worsens \( \sigma_z \). The best compromise for \( \lambda_{\text{eff}} \) was predicted \cite{1} by the simulations to be about 2/3 of the crystal length \( L_c \).

A recent experimental study \cite{3} with a set of polished YAP:Ce scintillators of dimensions 3.2 \times 3.2 \times 100 \text{ mm}^3 focused on methods of adjusting \( \lambda_{\text{eff}} \) by wrapping the bars with Teflon or by coating the crystal lateral surfaces with very thin metallic layers. In this paper, we simulate the optical processes in the crystal bars with Geant4 \cite{4} and compare the results to the experimental findings. The comprehension of the influence of the optical properties of the crystal surfaces on the light collection is an essential ingredient to optimize the detector performance.

The paper is organized as follows: Sect. II recalls the formulae which characterize the performances of the HPD-PET concept. Sect. III summarizes some of the experimental results reported in \cite{3}. In Sect. IV we discuss the Geant4 simulations which suggest an alternative approach to the problem of light collection, namely linear triangular engravings on the lateral surfaces of the polished crystal bars. The conclusions are summarized in Sect. V.

II. THE HPD-PET CONCEPT

The axial HPD-PET concept assumes that the measured pe yields \( N_1 \) and \( N_2 \) at the bar ends vary exponentially with the average path length of the scintillation light. For a single 511 keV \( \gamma \)-ray:

\[
N_1 = \frac{1}{2} \cdot N_0 \cdot \exp \frac{-z}{\lambda_{\text{eff}}}, \quad N_2 = \frac{1}{2} \cdot N_0 \cdot \exp \frac{-(L_c - z)}{\lambda_{\text{eff}}}, \quad (1)
\]

\[
N_{pe}(z) = N_1 + N_2, \quad (2)
\]

with \( N_{pe} \) being the total number of detected photoelectrons.

The axial coordinate \( z \) of the interaction point is derived

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from the relation:
$$z = \frac{1}{2} \left( \frac{\lambda_{\text{eff}} \ln N_f + I_c}{N_f} \right)$$
and its uncertainty, taking into account only the statistical error on $N_{1,2}$, is:
$$\sigma_z = \frac{\lambda_{\text{eff}}}{\sqrt{2N_0 / \text{ENF}}} \left( \exp \frac{z}{\lambda_{\text{eff}}} + \exp \frac{I_c - z}{\lambda_{\text{eff}}} \right)^{1/2}.$$  
(4)

The energy and time resolutions are respectively:
$$\sigma_E = \frac{\text{ENF}}{E} \oplus R_{\text{int}}, \quad \sigma_T = \frac{c}{\sqrt{N_{\text{pe}}} \oplus \sigma_c}.$$  
(5)

In the previous equations, $\text{ENF}$ is the excess noise factor [3] of the photodetector, $R_{\text{int}}$ the intrinsic resolution of the scintillator, and $c$ and $\sigma_c$ are constants to be determined experimentally. These equations clearly explicit that an increase of $N_0$ improves all the resolutions, while an increase of $\lambda_{\text{eff}}$ although improving $\sigma_E/E$ and $\sigma_T$ worsens $\sigma_z$.

### III. EXPERIMENTAL RESULTS

Fig. 1 shows a set of measurements [3] performed with polished YAP crystal bars of 10 cm length, wide $3.2 \times 3.2$ mm$^2$, and various treatments of their lateral surfaces. An effective light attenuation length of 20.8 cm was measured for a polished YAP crystal in air (full squares in Fig. 2). The energy resolution in the centre of the bar was found to be 8 mm (full squares in Fig. 2).

The energy resolution of the following intrinsic properties: light yield $N_{\text{ph}} = 18$ keV, intrinsic energy resolution $\sigma_E/\text{ENF} = 2.4\%$, refractive index $n_1 = 1.94$ at 370 nm. The bar lateral surface was assumed surrounded by air, or with a fraction ($f_2$ in Tab. 1) wrapped with a Teflon, allowed for the search of the best and practical technique to achieve the optimum detector performances.

A Teflon wrapping (full points) does not degrade the $N_0$ parameter [2-2$N_0$($z=0$)] with respect to a polished crystal. It only halves the attenuation length. But, as expected from Eq. 4, the resolution $\sigma$ is improved (Fig. 2).

A tuning of the light attenuation length could be obtained with metallic coatings (triangles in Fig. 1) in the range 11.9 to 3.9 cm [3] by adjusting the thickness of the vacuum deposited layers. However, because of their absorption (the refractive index is complex) an unacceptably large loss of the collected light was measured.

An even lower $\lambda_{\text{eff}}$ (~1.5 cm) could be obtained by roughing the crystal lateral surface with sand paper (stars in Fig. 1). But only a shorter crystal ($L_c=5$ cm), wrapped in Teflon, allowed the detection of correlated signals at the scintillator ends. The dependence of the yield on $z$ is no longer exponential.

### IV. GEANT4 SIMULATIONS

We discuss in this section the various optical parameters used in the Geant4 code to describe the light collection and their influence on the resolutions $\sigma_z$, $\sigma_E/E$. Once validated with experimental data, the Geant4 code provides an efficient tool for the search of the best and practical technique to achieve the optimum detector performances.

#### A – Principle and validation of the simulations

For the simulations we assumed YAP crystals with the following intrinsic properties: light yield $N_{\text{ph}} = 18$ keV, intrinsic energy resolution $\sigma_E/\text{ENF} = 2.4\%$, refractive index $n_1 = 1.94$ at 370 nm. The bar lateral surface was assumed surrounded by air, or with a fraction ($f_2$ in Tab. 1) wrapped with a Teflon, material, or coated. In this last case a complex refractive index ($n_2, k_2$) of the thick ($t$) coating is assumed. The PMTs coupled to the bar polished bases were simulated with a borosilicate window with a refractive index $n_w = 1.474$, an ENF of 1.2, and a quantum efficiency $\varepsilon_Q = 0.25$.

For some results Geant4 simulations were successfully cross checked against two other optical photon tracking codes: Litran [5], and Transport [6].

At each photon impact on the crystal lateral surfaces the following optical processes were considered [7] (see Fig. 3): absorption ($A$), transmission ($T$), reflection ($R$), diffusion ($D$), with a Lambertian distribution, and a possible smearing ($S$), i.e. a reflection $S_R$ or a transmission $S_T$ when the normal to the

### TABLE I

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_0$ (pe's)</td>
<td>963</td>
</tr>
<tr>
<td>$\lambda_{\text{eff}}$ (cm)</td>
<td>21.1</td>
</tr>
<tr>
<td>$A$ (%)</td>
<td>0</td>
</tr>
<tr>
<td>$D$ (%)</td>
<td>0</td>
</tr>
<tr>
<td>$n_2$</td>
<td>1</td>
</tr>
<tr>
<td>$k_2$</td>
<td>1</td>
</tr>
<tr>
<td>$f_2$</td>
<td>1</td>
</tr>
</tbody>
</table>

Polish: 963 21.1 0 0 1 1 1
Teflon: 1062 10.8 0.3 2 1.3 0 0.5
Cr: 820 9.9 0 0 1.87 2.69 1
Au: 767 5.1 0 0 1.7 1.88 1
local surface is rotated with respect to that of the average crystal surface. In this last case the rotation angle was randomly chosen from a Gaussian distribution with dispersion $\sigma_\alpha$. The backscattering was disregarded. Obviously, $A + R + T + D + S_R + S_T = 1$. $A$ and $D$ were varied independently of $n_1$ and $n_2$, the refractive indices of the crystal and its coating (or air). The reflection and transmission coefficients $R$ and $T$, or $S_R$ and $S_T$, were calculated according to the Fresnel relations assuming random polarization of the incident photons.

The yield of the indirect component $\text{yield}_{D + T + S_R + S_T}$ was calculated according to the Fresnel relations with the parameters listed in Table I. Of these, only $A, D, f_2$, and $f_3$ are free parameters determined from the fit procedures. The excellent agreement with the measured data proves the validity of the simulations. All results presented in the following figures are based on Geant4 simulations.

B– Influence of the optical parameters on $\sigma_z$ and $\sigma_{\sigma/E}$

The transmission of the scintillation light to the photodetector depends on the limit angle at the interface crystal-window $\theta_a = \sin^{-1}(n_w/n_1)$.

In long and thin crystals bars two components are transmitted to the photodetector:

- The direct component (the fraction of detected photons without reflections on the crystal lateral surfaces), dominant for scintillations at short distances from the window, is:

$$ f(\theta_a) = \frac{1}{4\pi} \cdot 2 \pi \cdot \int_0^{\theta_a} \sin \theta \, d\theta = \frac{1}{2} \left[ 1 - \cos \theta_a \right]. $$

(6)

where $\theta \leq \theta_a$ is defined by the distance to the PMT window.

The number of detected photoelectrons is

$$ N_{aa} = N_{ph} \cdot f(\theta_a) \cdot \epsilon_0. $$

(7)

The indirect component is the fraction of photons which propagates in the crystal bar by total internal reflection. It is limited to polar angles in the range from 0 to $\pi/2 - \theta_b$, with $\theta_b = \sin^{-1}(n_2/n_1)$ measured with respect to the normal of the window. The yield of the indirect component

$$ N_{aw} = N_{ph} \cdot f \left( \frac{\pi}{2} - \theta_b \right) \cdot \epsilon_0. $$

(8)

This is strictly correct only in the case of cylindrical crystal. For rectangular crystal the accepted angular range is somewhat larger, but the argument remains fully valid.

$\text{yield}_{D + T + S_R + S_T}$ decreases when $n_2$ increases, i.e. when a coating is used.

However, for $1 < n_2 \leq 1.25$, although the intensity of the indirect component decreases, the limiting factor is still the transmission at the PMT borosilicate window and the overall yield is therefore unchanged (see Fig. 4). On the contrary, for higher values of $n_2$ (1.5 in Fig. 4) the loss of light arriving at the end of the bar is dominant.

The behaviour is completely different with a sapphire window ($n_w = 1.793$). The transmitted photon flux starts to decrease when as soon as $n_2$ is larger than 1.

As shown in Fig. 4 $\lambda_{\text{eff}}$ is independent of $n_2$. However one observes at small distances a slight deviation from an exponential due to the detection of the direct component.

![Fig. 3. Schematic polar plot of the possible processes at the interface between the crystal ($n_1$) and the coated (or wrapped) lateral surface ($n_2$). Absorption ($A$) is not indicated in the figure.](image)

![Fig. 4. Photoelectrons $N_1$ detected on one bar end for scintillation at different $z$-positions in a polished YAP with a wrapping of the lateral surface with the indicated refractive indices. The lines are fits to the points according to Eq. 1.](image)

![Fig. 5. Photoelectrons $N_1$ detected on one bar end (upper panel) and z-resolution (lower panel) for scintillations at different $z$-positions in a YAP bar. The lateral surfaces are polished ($n_w = 1$). The different datasets correspond to photodetectors with different refractive indices of the window. The lines are fits to the points with Eq. 1 in the upper panel and with Eq. 4 in the lower one.](image)
values (full squares).

The influence of the absorption \((A)\) on \(N_1\) and \(\sigma_z\) is displayed in Fig. 7. Increasing \(A\) does not reduce \(N_0\) but lowers \(\lambda_{\text{eff}}\), improving \(\sigma_z\) which, however, gets saturated above 10%. These results, obviously, would improve with a sapphire window.

Fig. 6. Relative energy resolution, measured for 511 keV γ-rays detected in the centre of a YAP crystal long 10 cm, versus the refractive index of its lateral surface wrapping (circles), and of the photodetector windows (squares).

Fig. 7. Photoelectrons \(N_1\) detected (upper panel) at one bar end (photodetector with \(n_w = 1.47\)) and uncertainties in the scintillation position reconstruction (lower panel) for scintillations at different \(z\)-positions in a YAP bar with polished lateral surface \((n_2 = 1)\). The absorption parameter has been varied as indicated.

The consequences of the diffusion \((D)\) on \(N_1\) and \(\sigma_z\) are shown in Fig. 8. These are similar to those of the absorption but with an increase of \(N_0\). This is due to photons with polar angles above the limit angle at the interface that are lost in a polished crystal, but can acquire after diffusion a lower polar angle and, thus, be detected. For this reason, transport efficiencies greater than those calculated with Eq. 6 can be obtained. The \(\sigma_z\) improvement due to absorption and diffusion is counter-balanced with a worsening of the energy resolution, as observed in Fig. 9 for gammas interacting at the crystal centre. However the degradation is reduced with a diffusive coating due to the increase of \(N_0\).

Fig. 8. Photoelectrons \(N_1\) detected (upper panel) on one bar end (photodetector with \(n_w = 1.47\)) and uncertainties in the scintillation position reconstruction (lower panel) for scintillations at different \(z\)-positions in a YAP bar with polished lateral surface \((n_2 = 1)\) polished and diffusing the indicated percentages of the optical photon flux.

As shown in Fig. 10, the angular smearing effect destroys the exponential dependence of \(N_1\) on the \(z\) coordinate which is a requirement for the coordinate reconstruction by means of Eq. 3. Such an effect would seriously compromise the performance of the HPD-PET concept.

No variation of the \(N_0\) and \(\lambda_{\text{eff}}\) values has been found by varying the crystal cross section and its length \(L_c\) for polished YAP crystals in air coupled to a PMT with a borosilicate window.

However, an increase of the length worsens the resolution \(\sigma_z\) in agreement with Eq. 4 for a constant \(\lambda_{\text{eff}}\) value. The simulations suggest that a low percentage of photons undergoing Lambertian diffusion (obtainable, for example,
with a partial roughening of the lateral surfaces) is a good approach to improve $\sigma_z$. However, such a technique would be very challenging in view of a good reproducibility for the production of a large quantity of bars.

A very promising and practical method to obtain the required [1] performances seems a geometry related absorption of the lateral surfaces of the crystal bar. It could be implemented by triangular engravings (cuts) applied to the lateral surfaces of the polished crystal bars (see Fig. 11). The absorption probability $A$ is driven by the number of cuts and their depth. Various patterns have been simulated with Geant4. Technically, the pattern can be produced by laser etching followed by a chemical polishing [8].

Fig. 12 illustrates the performance which can be achieved for different parameters of the engraving. The method maintains the relation $N_1(z)$ perfectly exponential. In contrast to all other methods it allows to significantly improve $\sigma_z$ while $\sigma_E/E$ is practically unaffected. The resolutions are almost constant over the full bar length. A PET scanner with this performance would be a very competitive device.

V. CONCLUSIONS

In this paper we have discussed Geant4 simulations of the long and thin scintillator crystals bars to be used for the axial HPD-PET project.

These simulations have shown that the best matching of the refractive indices of crystal and the photodetector windows is, as expected, paramount to optimize the detected light yield, and consequently the energy and position resolution of the single gamma ray.

The various tested wrapping/coatings of the crystal lateral surface have contrasting results on the resolutions. Their behaviour is well reproduced by the Geant4 simulations and accounted for by the parameters $N_0$ and $\lambda_{eff}$, which are the key values characterizing the system crystal bar - photodetector.

The various optical parameters involved in the propagation of the photon flux have been parameterized and their respective contributions to the resolutions revealed by the simulations.

It appears that the best possible way to optimize the detector performances is to realize a controlled absorption of the crystal surfaces. An engraving technique has been proposed using laser etching and chemical polishing.

References