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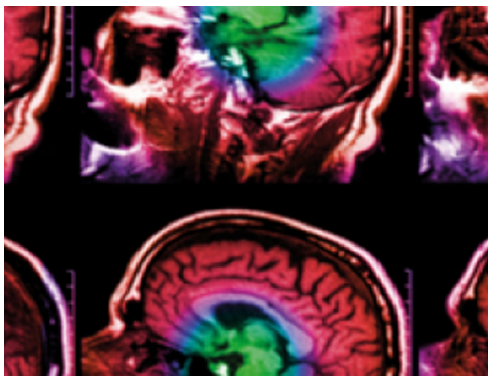
Achieving sub-100 ps time-of-flight resolution in thick LSO positron emission tomography while reducing system cost: a Monte Carlo study

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Achieving sub-100 ps time-of-flight resolution in thick LSO positron emission tomography while reducing system cost: a Monte Carlo study

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E-mail: stephan.walrand@uclouvain.be**Keywords:** positron emission tomography, time of flight, depth of interaction, optical Monte CarloSupplementary material for this article is available [online](#)

Abstract

Purpose. Evaluating the time-of-flight (TOF) resolution improvement that could be obtained using an easy crystal block modification which enables depth of interaction (DOI) assessment and simplifies the detector assembling process. **Method.** A fast optical Monte Carlo (MC) code was developed. The code was evaluated versus measurements of the energy resolution, number of detected scintillation photons and TOF resolution (TOFr) reported for different crystal photodetector setups. Then, MC simulations were performed for a modified crystal block section of $8 \times 8 \text{ mm}^2$ in which two partial saw cuts allow light sharing between four detector pixels with a strong dependence on the DOI. **Results.** Relative differences between MC simulations and reported measurements were always below 10% for any quantities. The simulations showed that the best TOFr was obtained by leaving the partial saw cuts empty. This feature results from the fact that for a slant angle lower than 56 degrees, the scintillation photons undergo a lossless total reflection at the L[Y]SO $\rightarrow$ air boundary, which is hardly achievable using a reflector material. According to the simulations, this approach allows a TOFr improvement from 163 ps to 90 ps full width at half-maximum using a 22 mm thick LSO 0.2%Ca:Ce crystal coupled to a FBK-NUV-HD silicon photomultiplier. **Conclusion.** Sub-100 ps TOFr using thick LSO crystal appears achievable using this simple crystal block modification. The method reduces by a factor of 4 the number of crystal pixels to be covered by a reflective material and afterwards joined together. As clinical positron emission tomography contains about 60 000 crystal pixels, this benefit would reduce the assembling cost.

1. Introduction

It is now well documented that improving the time-of-flight (TOF) resolution provides better clinical positron emission tomography (PET) imaging. In the last decade significant developments in crystal (Gundacker *et al* 2018) and in photodetectors (Gundacker *et al* 2016) have allowed researchers to reach 210 ps TOF resolution (TOFr) in a commercial LSO PET system (Reddin *et al*). However, continuing to narrow the TOFr without reducing the crystal thickness is hampered by the high refractive index (≈ 1.8) of Lu-based crystals (L[Y]SO).

Indeed, between two interactions, gamma rays travel in any material at the speed of light c , on the other hand scintillation photons travel L[Y]SO only with half that speed. Thus, according to whether the photoelectric effect location of the two opposing 20 mm thick L[Y]SO crystal blocks is closer to the front or to the back side, the detection time of a primary photon can be delayed by up to 106 ps. This delay is further magnified when crystal blocks are pixelated in order to improve the spatial resolution and the count rate capacity. As scintillation is isotropic, the probability is high, especially for small depth of interaction (DOI), that the first photons are emitted towards a crystal pixel surface. In this case, the photons will have to undergo several reflections before reaching the photodetector, further increasing their path and delaying their detections.

In order to correct the detection time, numerous solutions are under development to assess the DOI; see (Berg and Cherry 2018) for a detailed review. Examples of investigated solutions using pixelated blocks are multi-layer crystal (Furumiya *et al* 2014, Doroud *et al* 2019) and implementing a photodetector at both sides of the crystal (Kishimoto *et al* 2013, Derenzo *et al* 2015). Although promising, these solutions have the drawback of increasing the PET total cost. An elegant low-cost alternative was to implement light sharing between crystal pixels depending on the DOI, which was obtained by partially gluing the crystal pixels (Zhang *et al* 2019).

Similarly to the historic Exact HR PET system, we propose here to use partial saw cuts in a crystal block in order to allow scintillation light sharing between crystal pixels. However, contrary to the Exact HR PET the saw cuts are left empty and are set on the photodetector side. That makes the light sharing strongly dependent on the DOI. The aim of this study is to evaluate by Monte Carlo (MC) simulations the potential TOFr improvement allowed by this approach.

2. Material and method

2.1. Optical MC code design

A fast multi-threading optical transport MC code was written in Visual c++. The code was optimised in order to use the Intel Core streaming SIMD extensions (SSE) which allows four simultaneous 32-bit floating point operations. SIMD-oriented fast Mersenne twister random generators were used for uniform random drawing (Saito *et al* 2006) and specific random distributions were obtained from this uniform drawing using the rejection method (Press *et al* 1992).

In the TOF simulations, for each gamma ray the photoelectric DOI was drawn according to the crystal attenuation coefficient at 511 keV while the transverse position was uniformly drawn. For experiments on the light collection as a function of the DOI experiment, only the transverse position was drawn. The emission direction of the scintillation photon was drawn according to an isotropic distribution.

Photon transmission and reflection at the crystal and photodetector surfaces were drawn according to the Fresnel law. The crystal surface polishing imperfections were taken into account by randomly adding a Lambertian contribution to the Fresnel reflection and transmission with a probability $p = 1 - \text{polish}$, where $\text{polish} = 1$ corresponds to a perfectly polished surface and $\text{polish} = 0$ to a frosted surface. Reflection on the crystal covering material was randomly drawn according to the optical reflectance angular measurements made for commonly used reflectors (Janecek and Moses 2008).

The scintillation photon production and detection were randomly drawn according to the measured yield Y at 511 keV, crystal rise τ_r and decay τ_{d1} , τ_{d2} times for LYSO (Frach *et al* 2009) and for LSO (Gundacker *et al* 2020). The number of scintillation photons was drawn according to a Poisson distribution of mean Y and the emission time of each photon was drawn according to the distribution:

$$f(t) = \frac{\alpha e^{-t/\tau_{d1}} + (1 - \alpha) e^{-t/\tau_{d2}} - e^{-t/\tau_r}}{\alpha \tau_{d1} + (1 - \alpha) \tau_{d2} - \tau_r} \quad (1)$$

Where α is the abundance of the first decaying component, note that:

$$\int_0^{\infty} f(t) dt = 1 \quad (2)$$

And the rising behaviour, i.e. t much smaller than the decaying times, is:

$$f(t) \propto 1 - e^{-t/\tau_r} \quad (3)$$

Two photodetectors were simulated: the Philips silicon photomultiplier (SiPM) with a photon detection efficiency (PDE) = 26% (Frach *et al* 2009) and a timing resolution $J = 59$ ps full width at half-maximum (FWHM) (Haemisch *et al* 2012), and the FBK-NUV-HD with PDE = 59% and $J = 68$ ps FWHM (Gundacker *et al* 2020). The detection of a photon was drawn according to the PDE and a delay drawn according to a Gaussian distribution of FWHM = J was added to the photon entry time into the SiPM (Derenzo *et al* 2014).

Lastly, the detected photons were sorted according to the final detection time.

2.2. MC code validation

The MC code was tested versus the number of scintillation photons detected using LYSO blocks of various shapes and sizes, covered by specular or Lambertian reflective materials and coupled to different photodetector types. Afterwards, the TOFr of the state-of-the-art LYSO-SiPM was evaluated versus reported experiments.

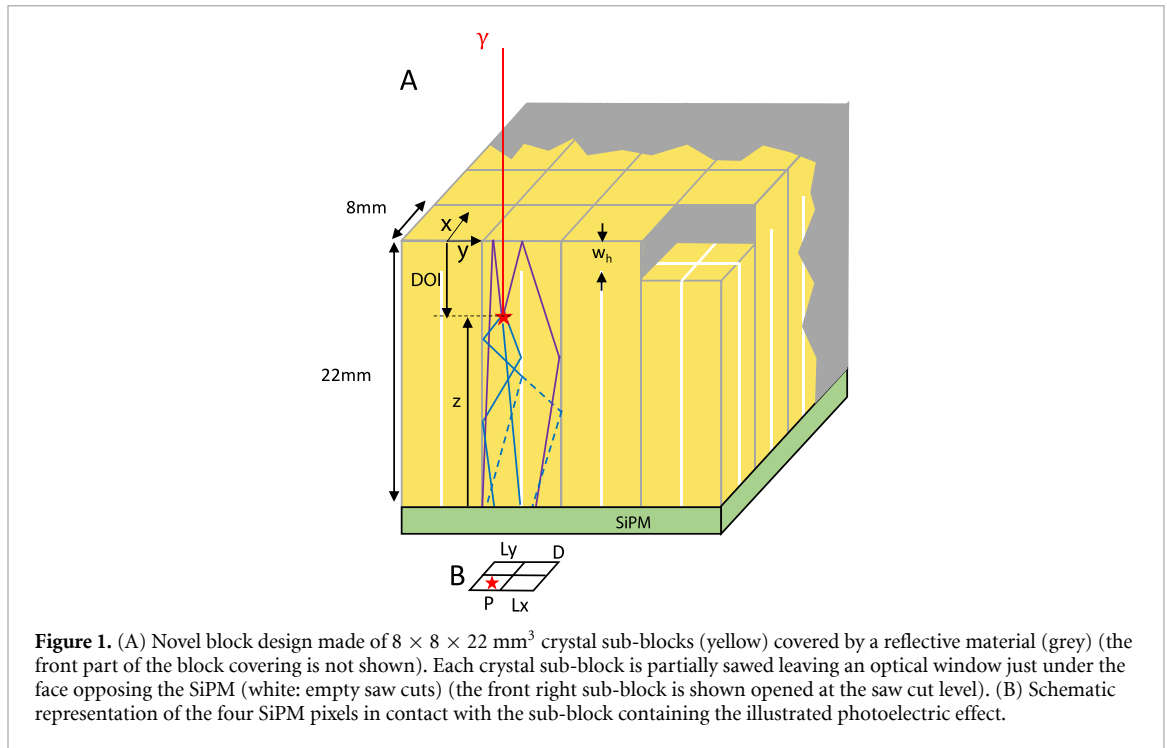


Figure 1. (A) Novel block design made of $8 \times 8 \times 22 \text{ mm}^3$ crystal sub-blocks (yellow) covered by a reflective material (grey) (the front part of the block covering is not shown). Each crystal sub-block is partially sawed leaving an optical window just under the face opposing the SiPM (white: empty saw cuts) (the front right sub-block is shown opened at the saw cut level). (B) Schematic representation of the four SiPM pixels in contact with the sub-block containing the illustrated photoelectric effect.

2.3. Novel crystal block design

Figure 1(A) shows the novel crystal SiPM block design which is made of $8 \times 8 \times 25 \text{ mm}^3$ crystal sub-blocks covered by a reflective material. Each crystal sub-block is partially sawed leaving an optical window of height W_h just below the side opposing the photodetector. Depending on the DOI, the scintillation photons are more or less spread on the four $4 \times 4 \text{ mm}^2$ SiPM pixels in contact with the crystal sub-block (figure 1(B)). No reflective material is inserted in the saw cuts. As the LSO and LYSO refractive index is around 1.8, for a slant angle lower than 56 degrees ($90 - \arcsin(1/1.8)$) all photons undergo a lossless total reflection, otherwise they undergo a transmission or a reflection according to the Fresnel law (blue dashed lines in figure 1(A)).

2.4. DOI and TOF assessment

The DOI was modelled as:

$$DOI = a_0 + a_1 \frac{L_x + L_y}{P} + a_2 \frac{D}{P} + a_3 \left(\frac{L_x + L_y}{P} \right)^2 + a_4 \frac{L_x + L_y}{P} \frac{D}{P} + a_5 \left(\frac{D}{P} \right)^2 \quad (4)$$

where P , L_x , L_y , D are the number of photons detected in the four SiPM pixels in front of the crystal sub-block (figure 1(B)).

The corrected TOF_c using the measured DOI is:

$$TOF_c = TOF + (DOI - T_c) \frac{n_r - 1}{c} \quad (5)$$

where T_c and n_r are the crystal thickness and refraction index, respectively, while c is the speed of light in vacuum.

The window height W_h and the parameters a_i were fitted in order to get the best TOF assessment and not the best DOI assessment. This choice allows taking into account that the first detected photons often undergo several reflections resulting in a smaller apparent DOI. For this optimisation 30 000 MC simulations were performed for a DOI ranging from 0 mm to 22 mm in 1 mm steps.

Afterwards, a second set of parameters a_i was optimised in order to get the best DOI assessment, but using the window height W_h optimised for the TOF assessment. This second set also allowed us to get an accurate DOI to correct for parallax effects.

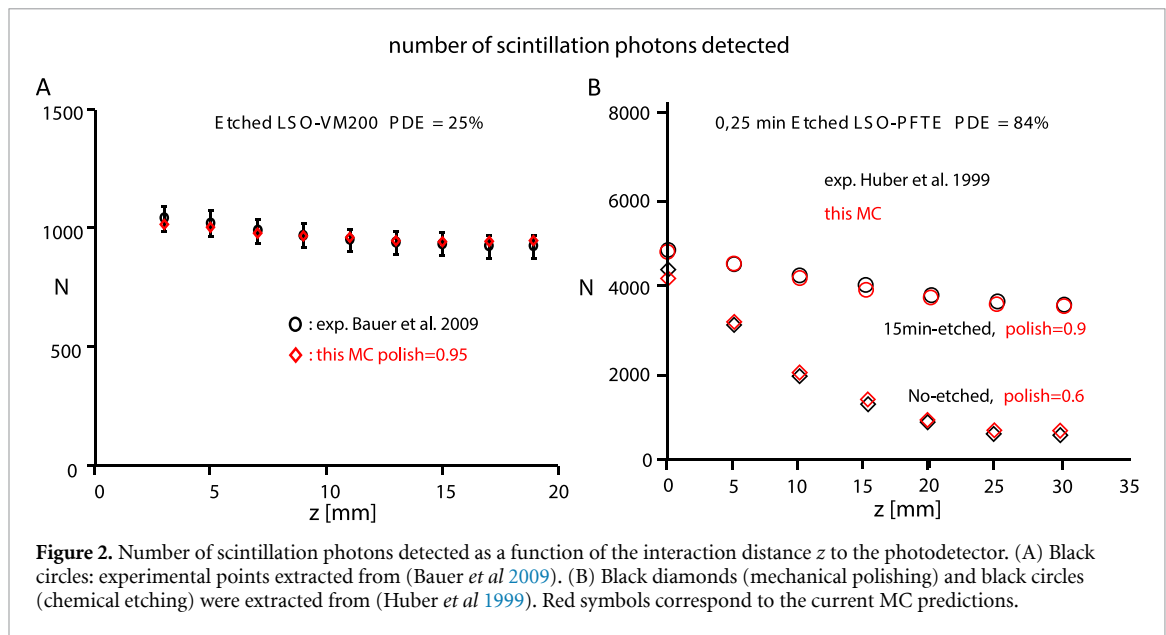


Figure 2. Number of scintillation photons detected as a function of the interaction distance z to the photodetector. (A) Black circles: experimental points extracted from (Bauer *et al.* 2009). (B) Black diamonds (mechanical polishing) and black circles (chemical etching) were extracted from (Huber *et al.* 1999). Red symbols correspond to the current MC predictions.

Table 1. MC code evaluation versus reported experiments for the energy resolution and TOFr (Degenhardt *et al.* 2009, 2012).

	Experiments	Our MC code
Energy resolution	10.7–12.1%	10.5%
TOFr 1 photon triggering	240–283 ps	262 ps
TOFr 2 photon triggering (Philips Vereos)	316 ps	321 ps

3. Results

3.1. MC code validation

Figure 2(A) shows the MC code evaluation in photon counting experiments (Bauer *et al.* 2009) using a $2.5 \times 2.5 \times 20$ mm³ chemically etched LSO coupled to a R8619 photomultiplier tube (PDE = 25%). The crystal was covered by the pure specular reflective material VM 2000 (Janecek and Moses 2008).

Figure 2(B) shows the MC code evaluation in photon counting experiments (Huber *et al.* 1999) using a $2.2 \times 2.2 \times 20$ mm³ mechanically polished or chemically etched LSO coupled to a photodiode (PDE = 84%). The crystal was covered by specular Lambertian reflective PTFE (Teflon[®]) tape (Janecek and Moses 2008).

In both studies, different photoelectric distances z to the photodetector were investigated by moving a collimated ⁶⁸Ge source along the crystal.

The present MC simulations using polish values of 0.6 and 0.95 are in good agreement with mechanically polished and perfectly etched crystal surface acquisitions, respectively.

Table 1 shows the MC code evaluation for the energy resolution and TOFr measurements using a $4 \times 4 \times 22$ mm³ LYSO from different vendors (Frach *et al.* 2009, Degenhardt *et al.* 2009, 2012). The crystals were mechanically polished, i.e. MC polish = 0.6, covered by three layers of Teflon[®] tapes and coupled to the Philips SiPM using one or two photons for the time stamp triggering.

3.2. Novel design: scintillation photon spreading

Figure 3 shows the light spreading between the four photodetector pixels in front of the crystal sub-block (figure 1(B)) as a function of the DOI. Note that the pixel P aligned with the photoelectric effect always gets the higher number of counts for any DOI allowing to transversally localise the gamma interaction in the crystal block.

3.3. Novel design: DOI and TOFr assessment

The window height giving the best TOFr was $W_h = 3.0$ mm.

Figure 4 shows the standard variation σ of the DOI using the parameters a_i optimised for the DOI assessment and the window height optimised for the TOFr. The poor σ for small DOI is explained by the fact that in this optical window region the light sharing does not strongly depend on the DOI (see figure 3).

Table 2 shows the TOFr for the conventional design and the novel block design with empty saw cuts simulated for three different 22 mm thick crystals mechanically polished (polish = 0.6) and two SiPMs using

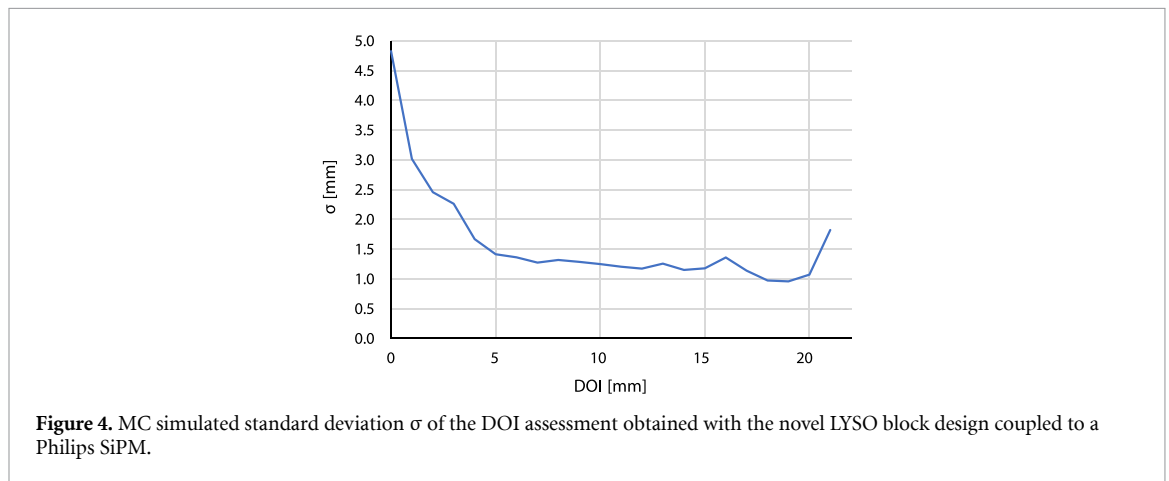
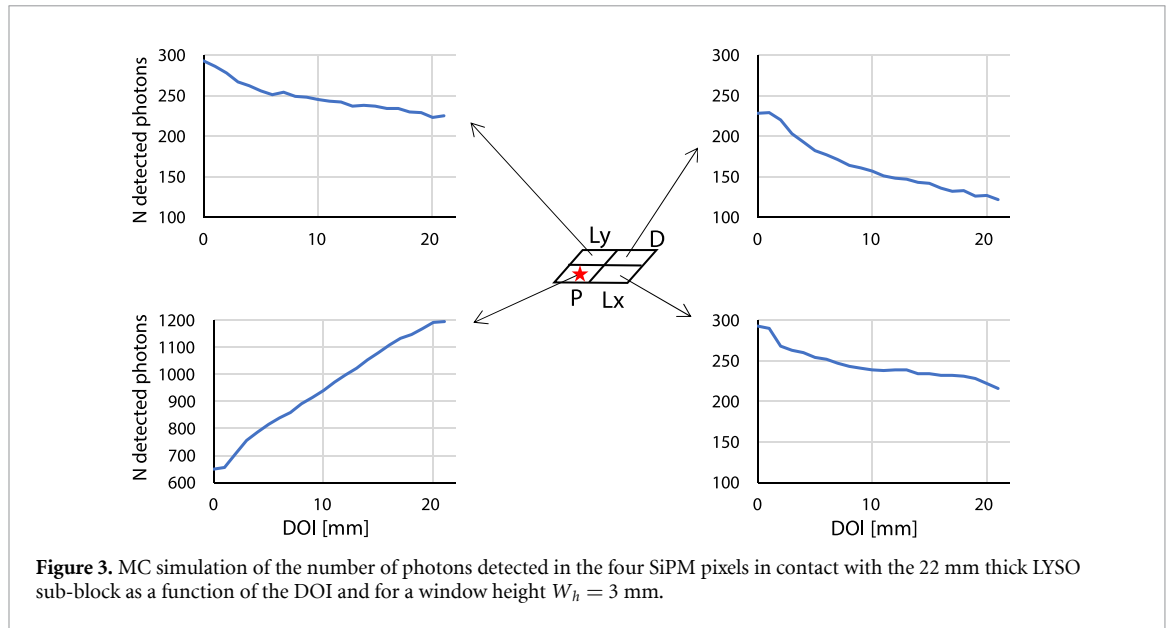


Table 2. Obtained TOFr FWHM for the conventional design and for the novel block design with empty saw cuts.

Crystal	Yield [/511 keV]	τ_r [ps]	$\tau_{d1}; \tau_{d2}$ [ns]	$\alpha; 1-\alpha$ [%]	SiPM	PDE [%]	J [ps]	Conv. TOFr [ps]	Novel TOFr [ps]
LYSO	16 000	2	37	100	Philips	26	59	308	204
LSO 0.4%Ca:Ce	16 400	10	8;32	5;95				277	179
LSO 0.2%Ca:Ce	20 000	9	10;35	5;95	FBK NUV HD	59	68	170	99
								163	90

the parameters a_i optimised for the TOFr assessment. The crystal sub-blocks were wrapped with four Teflon[®] layers. The optimal window height W_h was 3 mm, with a small TOFr variation of about 1 ps for W_h ranging from 2.5 mm to 3.5 mm. The number of photon triggering was 2.

The computation time using eight parallel threads running on an Intel Core i7-1065G7 10th generation clocked at 1.3 GHz was about 7 min for 30 000 photoelectric effects together with a scintillation yield of 20 000/511 keV.

In table 2 the saw cuts were left empty; simulation with the saw cut filled with a reflective material showed a TOFr degradation of 23 ps for the third setup, i.e. a TOFr of 113 ps in place of 90 ps. Lastly, TOFr assessment performed using the parameters a_i optimised to get the best DOI assessment resulted in a TOFr degradation of 49 ps. Figure 5 shows the mean DOI assessment for the third setup as a function of the actual DOI using the parameters a_i optimised for the DOI or for the TOFr assessment.

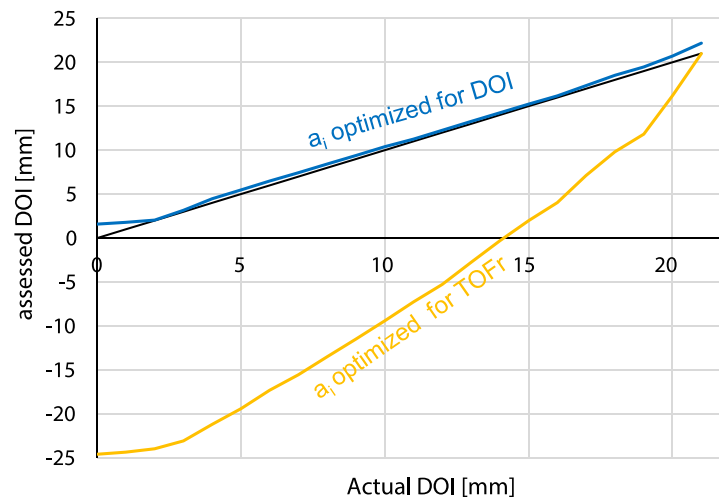


Figure 5. DOI assessment averaged on 30 000 simulations for the 22 mm thick LSO and FBK NUV HD setup as a function of the actual DOI and using the parameters a_i optimised for the DOI (blue curve) or for the TOF (yellow curve) assessment. The black line is the identity. Due to reflections increasing the path length, the photon arrival time corresponds to an apparent DOI (yellow curve) smaller than the actual one (black curve).

4. Discussion

The present study shows that a TOFr improvement from 163 ps to 90 ps is possible in thick crystal by an easy modification of the block crystal, simply consisting of partially sawing the block. The resulting scintillation light sharing between four pixels allows an accurate assessment of the DOI (figure 4) resulting in the above-mentioned TOFr improvement. The final TOFr using state-of-the-art crystal and SiPM is better than 100 ps FWHM (table 2).

Partial saw cuts in crystal is an old process which was already applied for the pioneer Exact HR PET system. The current process is still easier as there is no need to fill the saw cuts with a reflective material such as for the Exact HR PET. Besides the simplicity, there are other benefits in leaving the saw cuts empty: for slant angles below 56 degrees the photons undergo a lossless total reflection which is hardly attainable with conventional reflector materials (Harmon *et al* 2019). The fraction of photons crossing the saw cuts for larger angles is not an issue: it just participates in the light sharing.

The good DOI assessment with the parameters a_i optimised for this task appears amazing. It results from the fact that the number of detected photons in the primary pixel increases with the DOI while it is the opposite for the three adjacent pixels (figure 3). For small-animal non-TOF PET systems, it should even be possible to improve this DOI assessment by optimising the window height specifically for this task.

For TOF assessment, the simulations show that it is much better to optimise the parameters a_i not to get the best actual DOI assessment, but directly to get the best TOF assessment using equations (4) and (5). This feature results from the fact that, often, the first detected photons have already undergone several reflections, resulting in a delay corresponding to an apparent DOI smaller than the actual one. In a real TOF-PET building, the a_i parameters should preferably be optimised to get the best TOF assessment from photon counting using a positron source located at the PET ring centre, where the difference of the actual TOF of the two gamma rays is known to be null.

It could also appear amazing that the slower rising LSO crystal and the SiPM with the worse timing resolution obtained the best TOFr. That results from the major role played by the number of detected photons N as shown by intensive MC simulations (Derenzo *et al* 2014). This study provides an accurate but sophisticated formula predicting the TOFr. For L[Y]SO crystals coupled to SiPM this formula approximately reduces to (see supplementary file available online at stacks.iop.org/PMB/65/205009/mmedia):

$$TOFr \approx 2.20 \sqrt{\frac{\tau_d (\tau_r + d + 0.95 J)}{N}} \quad (6)$$

where d is the photon time dispersion in the crystal. As N is proportional to the scintillation yield, the prediction of the TOFr for LSO 0.2%Ca:Ce-FBK-NUV-HD can be derived from that obtained for LSO 0.4%Ca:Ce-FBK-NUV-HD using equation (6), i.e.:

$$170 \sqrt{\frac{16400}{20000} \frac{35}{32}} = 161 \quad (7)$$

This value is perfectly in line with the MC simulation (see table 2), showing that our MC code behaves similarly to that of Derenzo *et al*. Equation (6) enables a fast estimation of the error propagation: due to the square root dependence, the relative variation of the crystal decay time or of the number of photons detected is reduced by half in the final TOFr. The impact on the TOFr of variations on τ_r and on J is further dumped by the addition of the dispersion time in the crystal d .

Compared to the light sharing method previously proposed in (Zhang *et al* 2019), the present one does not use a reflective material between the crystal pixels sharing the light. MC simulations showed that the lossless total reflection from high to low refractive index transition, i.e. L[Y]SO $\rightarrow$ air, provided an additional TOFr improvement of 23 ps. Furthermore, the present method also has the benefit of reducing the manufacturing cost. Indeed, it is easier to saw four partial cuts and leave them empty, rather than perform four total cuts, partially cover the four resulting crystal pixels by a reflective material, and lastly glue them together. Let us recall that human PET rings are made of several tens of thousands of such crystal pixels. In fact by reducing by a factor of 4 the number of crystal pixels to be covered by a reflective material, this method would likely reduce the ring assembling cost versus conventional PET.

5. Conclusion

Sub-100 ps TOFr using thick LSO crystal appears achievable using this simple crystal block modification. The method reduces by a factor of 4 the number of crystal pixels to be covered by a reflective material and afterwards joined together. As clinical PET contains about 60 000 crystal pixels, that would reduce the assembly cost.

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