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Exploring light confinement in laser-processed LYSO:Ce for photon counting CT application

L Bläckberg¹, S Sajedi¹, S Mandl^{1,2}, A Mohan^{1,3}, B Vittum^{1,3}, G El Fakhri¹, H Sabet¹

¹Gordon Center for Medical Imaging, Department of Radiology, Massachusetts General Hospital & Harvard Medical School, Boston, MA, USA

²McGill University, Montreal, Canada

³Northeastern University, Boston, MA, USA

Abstract

With the goal of developing a low-cost scintillator-based photon counting detector (PCD) with high dose efficiency suitable for CT, the light transport characteristics in LYSO:Ce detectors containing Laser Induced Optical Barriers (LIOB) are simulated. Light confinement and light collection efficiencies (LCE) are studied for a variety of optical barrier patterns and properties (refractive index (RI) and barrier/crystal interface roughness). Up to 80% confinement is achievable with a simple pixel pattern with one barrier wall separating each pixel coupled one-to-one to a photodetector (PD) pixel. Confinement is heavily dependent on barrier properties, and rough interfaces and higher RI results in increased cross-talk. Three approaches to enhance performance beyond the basic pattern are explored: 1) Multiple barrier walls separating each crystal pixel. 2) Introduction of long and short range confinement by having multiple crystal pixels per PD pixel. 3) Combination of LIOB and Laser Ablation. 1) Is effective for rough interfaces where confinement can be increased by up to 24% for double compared to single walls. 2) Results in high confinement in the pixel centered on the PD pixel, but lower confinement closer to the PD edge. This feature may be explored to achieve spatial resolution beyond the PD pixel size using light sharing based positioning algorithms. 3) Can increase confinement for smooth interfaces using a smooth ablation in the bottom part of the crystal. A general trend across all configurations is a trade-off between light confinement and LCE. The LCE attainable is found comparable to that for mechanically pixelated arrays. While the confinement achievable with LIOB is always lower compared to a mechanically pixelated array, the former may offer a high level of flexibility in terms of detector design. This, in combination with the possibility to fabricate sub-mm pixels in a cost-effective manner, makes LIOB a promising technology for scintillator-based PCDs.

1 Introduction

Computed Tomography (CT) together with Magnetic Resonance Imaging (MRI), are the main modalities that can provide detailed 3-dimensional imaging of patient anatomy and have many important applications in diagnostic imaging and radiation therapy planning. While CT is faster and less expensive than MRI, it suffers from radiation exposure to the

patient and poorer soft tissue contrast. The latter issue has over the past years become an active area of research involving advancements in both image reconstruction and hardware. These include the development of dual-energy CT (DECT), or more broadly spectral CT, using conventional energy integrating detectors (EID) and energy-resolving photon counting detectors (PCD) [1]. DECT has shown promise to reduce patient dose [2], improve contrast, reduce beam hardening and metal artifacts [3] and improve material differentiation capabilities [1, 4–6].

EIDs used in conventional CT scanners measure the flux of X-ray photons transmitted through the body by summing the energy of all X-rays deposited in each detector pixel, without providing any information regarding the energy of individual X-rays. This approach results in that higher weight is given to the X-ray photons with larger energy compared to those with lower energy. PCDs on the other hand, measure the energy of each incident X-ray photon and categorize the events into (often adjustable) energy bins. This added information regarding the X-ray flux can lead to improved image resolution, improved contrast to noise ratio (CNR), lower noise, dose reduction, and less artifacts [7–11]. These benefits, in combination with enhanced material decomposition capabilities, open up for the possibilities of quantitative CT, accurate K-edge imaging and simultaneous imaging of multiple contrast agents [11–15]. Due to these advantages, which may come with substantial clinical benefits, a lot of effort has been put into the development of PCDs. However, while PCDs have been acknowledged for their fundamental advantages, the technology is still inaccessible at reasonable cost for clinical settings at standard X-ray flux rate [11, 16].

To the best of our knowledge, PCDs in CT applications have been exclusively referred to as semiconductor detectors (a.k.a direct conversion detectors). This is in contrast to EIDs that are almost exclusively scintillator-based, also referred to as indirect conversion detectors when compared with semiconductors. Scintillators have however been used for decades as photon counting detectors in nuclear imaging systems such as gamma-cameras, Positron Emission Tomography (PET), and Single Photon Emission Tomography (SPECT) systems. However, reasons such as the extra step of converting scintillation light to an electric signal, a relatively slow detector response, detector pixel size inaccuracy and escalating cost for fabricating detector arrays with small pixel dimensions may have prevented the use of scintillators as PCD in CT.

One major challenge that any PCD for clinical CT is facing is photon counting capability at high X-ray flux rate, as in CT the un-attenuated rate can reach 10^9 cps/mm² at the detector plane. It should be noted that by using a dynamic bowtie filter and a patient present in the scanner FOV, this rate is however reduced to 10^5 - 10^8 cps/mm² [16]. In this regard, Silicon (Si) detectors, thanks to their fast charge mobility, are an excellent choice for PCD for low energy X-rays [17, 18], but in a conventional setup they fall short for mid- to high-energy X-rays as the absorption efficiency rapidly drops due to the low Z (atomic number) of Si (see Figure 1). In principle one may increase the detector thickness to increase the absorption efficiency, but such approach comes with issues related to charge sharing and degraded energy resolution due to larger charge cloud, need for increased bias voltage and cost. An alternative solution to this limitation is to arrange the detectors in edge-on configuration pursued by some research groups in order to preserve spatial and energy resolution with high

absorption efficiency [19, 20]. However, this configuration can lead to substantially lower geometrical fill factor (and geometric sensitivity) depending on the thickness of readout electronic board and the spacing between detector boards, unless the detectors are arranged in more complex layered configurations as proposed in [20]. Also, direct exposure of the electronics in edge-on configuration may result in electronic component fatigue and damage. We believe these limitations were the key to explore other semiconductor materials with higher density and higher effective Z such as Cadmium Telluride (CdTe) [21–25] and Cadmium Zinc Telluride (CZT) [23, 26–28]. These materials are actively being studied for use as PCDs, as they have higher absorption efficiency and hence are more straightforward to use also for higher X-ray energies (see Figure 1). These two materials do however have significantly lower charge mobility compared to Si, which results in pileup issues at lower count rates, and as the technology is not as mature as Si the detector fabrication still comes with a number of technological challenges. As a consequence, both CZT and to some extent CdTe are expensive, which makes scaling to whole body scanners challenging from a cost-perspective. The main hurdles for wide-spread use of PCDs in clinical settings are the cost of raw PCD-grade CZT material, detector fabrication yield and pixel-to-pixel performance uniformity in the detectors.

One way of reducing the count rate burden per electronic channel in any PCD, is to make the detector pixels smaller and in that way reduce the flux-rate per channel. For pixels with $0.2 \times 0.2 \text{ mm}^2$ cross-section, the upper limit of 10^8 cps/mm^2 count rate would be reduced to $4 \times 10^6 \text{ cps/pixel}$, which is easier to achieve from a technical point of view. As the semiconductor industry is very mature, fabrication of anode patterns in semiconductor-based PCDs to create detectors with $<0.5 \text{ mm}$ pixel size is not challenging, and such fine structures are well within reach, at least for Si detectors. There are still some technical challenges facing CdTe and CZT PCDs such as bump-bonding problems when the pixel size is small and pixel-to-pixel uniformity, but the semiconductor industry has the *enabling technologies* to improve upon these shortcomings.

The fact that scintillator material is at least an order of magnitude cheaper than semiconductors like CZT, and new techniques for developing fine-pitched scintillator arrays, has motivated us and other groups to revisit the scintillator-based PCD (ScPCD) concept. The bottleneck for development of a ScPCD for CT has been the need for very fine pixelation, which has not been possible using standard mechanical array fabrication techniques. While conventional microcolumnar and some recent high resolution scintillator developments [29–32] have not been shown capable of high rate CT applications, there are other recent *enabling technologies* for fine-pitch scintillator array fabrication using laser beams that have shown promise [33–39].

Given that scintillators respond to radiation by emission of optical scintillation photons that are subsequently collected by a photodetector, the performance of a scintillator-based detector system is governed by the light transport in the detector. It is apparent that the building block of a ScPCD is to use one-to-one coupling between the photodetector and the scintillator pixel aiming at complete optical isolation among the pixels to reduce cross-talk, as such has a negative effect on spatial resolution, energy resolution, noise characteristics and count rate capability. Ideally one would want complete light confinement within the

scintillator pixel in combination with complete light collection efficiency as the gold standard. To the best of our knowledge, there is no literature comparing the potential performance of these new laser-processed detectors with the industry standard mechanical arrays. This has motivated us to do a head-to-head detector-level comparison of laser-based scintillators with that of an ideal case of a mechanically pixelated scintillator array as the industry standard.

2 Materials and methods

Scintillators respond to X-ray interactions by emission of optical photons, which are collected by a photodetector that generates an electrical signal *proportional* to the energy of the incident X-ray. If operated in pulse mode, as opposed to integration mode that is used in conventional CT, each pulse is analyzed and a pulse height spectrum can be generated similar to in a semiconductor detector.

In this paper we present a simulation study of the light transport in scintillator arrays produced using laser-based scintillator array fabrication techniques, as well as standard mechanical pixelation. The main purpose of this work is to investigate and compare the light confinement and light collection efficiency attainable in each of these configurations. As the performance of any scintillator-based detector is determined by the light transport in said detector, and the performance of a PCD for CT is highly dependent on the inter-pixel cross-talk, this study serves as a first step towards determining the feasibility of a ScPCD for CT.

In the following sections we describe the conceptual design of a scintillator detector configured as a PCD for CT (Section 2.1), outline the details of the detector types we have simulated in this paper (Section 2.2), the simulation parameters used (Section 2.3) as well as the overall setup of our simulations (Section 2.4).

2.1 Conceptual design of scintillator-based PCD

The conceptual design of a potential ScPCD contains a finely pixelated scintillator detector array, where each crystal pixel is coupled one-to-one with a photoconversion step and associated Application Specific Integrated Circuit (ASIC) pixel, as illustrated in Figure 2. Among various approaches, one is to incorporate a photodiode inside the ASIC pixel itself, which also contains a charge-sensitive preamplifier, a shaping amplifier with programmable peaking time, a number of energy windows (for example 3 or 4) and their associated counters (see Figure 2 a). Alternatively, the photodetector can be a Silicon Photomultiplier (SiPM) placed outside the ASIC pixel as shown in Figure 2 b).

The scintillator material we are currently exploring for this application is Cerium doped Lutetium Yttrium Oxyorthosilicate (LYSO:Ce). LYSO:Ce is a fast and bright scintillator with high stopping power and the mainstay detector material for PET. The stopping power exceeds that of both CdTe and CZT (see Figure 1) and 2 mm thickness is enough to stop virtually 100% of 70 keV and 87.9% of 140 keV X-ray photons. LYSO:Ce has a decay time of ~40 ns, and with a 5th order shaping amplifier 95% of the light should be collected with a peaking time of ~140 ns [41, 42], which would lead to a theoretical count rate capability of ~7 MHz. Taking into account SNR and Equivalent Noise Charge (ENC) this value would

likely be reduced to ~1 MHz. As mentioned, a PCD for CT needs to cope with 10^5 - 10^8 cps/mm², resulting in a target maximum count rate of 4×10^6 cps/pixel for pixels with 0.2 mm pitch. One can use approaches such as using shorter peaking times, or operating the detector in energy integrating mode at high fluxes and photon counting mode in low fluxes, to enable higher count rate.

A major challenge to overcome in order for a ScPCD to be practical is the fabrication of the scintillator array itself, given the thin pixels with small cross-section needed. The industry standard for scintillator pixelation involves mechanical cutting, polishing, and insertion of reflectors to confine the scintillation light, which becomes labor intensive and cost-prohibitive as the pixels become smaller. This is especially true for LYSO:Ce crystals, as well as many other attractive scintillator materials, which are hard and brittle resulting in a low material yield. In this manuscript we are focusing on alternative scintillator array fabrication techniques involving laser beams.

There are a number of laser-based techniques being explored for scintillator processing for different applications, including Laser Ablation (LA) [43, 44], Laser Induced Optical Barriers (LIOB) [33–36, 45–47], and the similar technique of Sub-Surface Laser Engraving (SSLE) [37, 38, 48]. Common for all the above-mentioned techniques are that they make use of a high power pulsed laser to create structured scintillators in order to achieve light confinement.

In LA the laser is focused on the crystal surface to create a cut that can subsequently be filled with reflector material. One limitation of the LA technique is that the created cut has an inherent V-shaped profile, which makes the technique limited to thin detectors. For LIOB and SSLE, on the contrary, the laser is focused inside the crystal bulk where the energy transfer results in a permanent modification of the crystal structure. In SSLE the result is the formation of micro-cracks on which the optical scintillation photons can scatter. In LIOB on the other hand, the crystal structure is locally modified to create so-called optical barriers, which have a refractive index lower than that of the surrounding crystal bulk. The optical barriers can be placed in virtually any pattern inside the crystal and will redirect the scintillation light and allow for control of the light spread in the detector. The properties of the barriers (i.e. size, shape and refractive index), can be controlled to some extent by tuning laser parameters during processing [39]. The technique is heavily material dependent but once optimized for a given material it can allow for cost-effective production of scintillator arrays due to high material yield in an automated process.. Both the LIOB and the SSLE techniques have been used for PCD fabrication in nuclear imaging for both PET [36, 38, 45, 47, 48] and SPECT [34]. We have previously shown that down to 0.25 mm pixels can be achieved in thin LYSO:Ce samples suitable for CT [39].

2.2 Simulated detector configurations

A mechanically pixelated array, a monolithic crystal and a variety of laser-processed LYSO:Ce detectors have been simulated using the Monte Carlo code DETECT2000 [49]. Noteworthy that simulating the monolithic crystal is for comparison and code validation and not for practical use in PCD. In all cases the overall detector dimensions were kept constant at $9.4 \times 9.4 \times 2.0$ mm³. The cross-section was chosen to match the dimensions of an 8×8

Multi-Pixel Photon Counter (MPPC) array with 1.2 mm pitch and $1 \times 1 \text{ mm}^2$ active pixel area. The implementation of this photodetector is described further in Section 2.3.2. It should be noted that the simulated pixel size is larger than what we are aiming for in a final PCD design, which is somewhere between 0.2 and 0.5 mm. However, as there are no photodetectors available on the market with pixels smaller than 1 mm, for clarity we have chosen to simulate pixels of this size in order to facilitate coupling of the simulations to experiments. In all cases the 5 sides of the detector that are not coupled to the photodetector were wrapped in an external diffuse reflector with a reflection coefficient of 0.98, corresponding to 3 layers of Teflon tape [33, 50]. The exit surface of the detector connected to the photodetector array was polished in all cases.

2.2.1 Mechanically pixelated array—The mechanically pixelated array was simulated as an array of 8×8 individual pixels, each coupled one-to-one with an MPPC pixel. The pixel pitch was 1.2 mm, and the reflector thickness 0.2 mm, in order to match the MPPC array. The reflectors were modeled as external diffuse reflectors with a reflection coefficient of 0.98, and no photon transport within the reflector material was simulated. The outer surfaces of each pixel were simulated as either polished or unpolished.

One difficult task in fabrication of mechanically pixelated arrays is the insertion of reflectors in between the pixels. This procedure becomes especially challenging as the pixels become smaller and the crystals thinner. For this reason, we have studied arrays where the reflectors are not covering the full pixel length, in order to estimate the effect on light collection, as well as to have a more realistic setup for comparison with the laser-processed detectors. In this regard we simulated 4 different configurations: reflectors along the whole pixel thickness, reflectors missing in the bottom 100 μm of the detector (close to the MPPC), reflectors missing in the top 100 μm (opposite to the MPPC), and reflectors missing in both the top and bottom 100 μm of the crystal.

2.2.2 Monolithic crystal—A monolithic $\text{LYSO}:\text{Ce}$ detector was studied in two configurations, with polished and unpolished outer surfaces. A monolithic crystal offers limited transversal resolution making it unsuitable for the present application. Hence, this detector type was studied for comparison purposes as it provides the expected performance in the absence of any light confining structures.

2.2.3 Laser-processed crystal—For the laser-processed detectors a range of optical barrier patterns were simulated as shown in Figure 3. The barrier RI and roughness of the barrier/crystal interface was varied per each optical barrier pattern, given that the properties can be controlled to some extent by tuning laser parameters during processing. All patterns are based on simple pixel-like structures, similar to a standard mechanically pixelated array.

2.2.3.1 Single barriers with one-to-one coupling to the MPPC pixels: The simplest and most straightforward pattern is a pixel pattern with one single wall of optical barriers separating each pixel-like volume in the crystal. For this configuration the width of the optical barrier wall (d_{OB}) as well as the width of the MPPC dead space (d_{DS}) was varied. This allowed the investigation of the impact of overlap between the crystal active area and

the MPPC dead space, as well as between the optical barriers and the active MPPC area. The three main varieties of this configuration are described in Figure 3 part 1.

2.2.3.2 Multiple barriers: Secondly, in an attempt to increase the confinement beyond the basic single wall pattern, multiple barrier walls were simulated between each pixel-like volume,. Here the cases of double and triple barrier walls were studied. For each configuration the optical barrier width was kept constant at 50 μm , while the spacing between the barrier walls was varied to simulate different types of optical barrier / MPPC dead space overlap, as illustrated in Figure 3 parts 2 and 3. The total barrier width is here defined as $d_{\text{TOT}} = n_{\text{OB}}d_{\text{OB}} + (n_{\text{OB}} - 1)d_{\text{LS}}$, where d_{LS} is the width of the spacing between the optical barrier walls.

2.2.3.3 Multiple crystal pixels per MPPC pixel: We further created a pattern with multiple equally sized crystal pixels on top of each MPPC pixel. This is one variety of the multi barrier wall pattern, but each crystal pixel will have different number of walls separating it from the next MPPC pixel. This characteristic may be explored for event positioning as the cross-talk between MPPC pixels will be dependent on the interaction location. For this configuration the cases of 3×3 and 5×5 crystal pixels per MPPC pixel were simulated, as illustrated by the schematic drawing in Figure 3 part 4.

2.2.3.4 Combination of LIOB and laser ablation: Finally, a combination of the LIOB and the laser ablation (LA) techniques was explored. With laser ablation detector material is removed from the crystal rather than modified as for LIOB. The same type of laser system can be used for both techniques, and hence the added complexity of fabrication of this type of detector is minimal compared to LIOB only.

The combination of LA and LIOB would also be an efficient way to mitigate technical difficulties and limitations inherent to each of the two techniques. Technically, with laser ablation one should be able to achieve complete isolation between pixels, as in a mechanically pixelated array. However, the drawback of this technique is the inherent V-shape profile of the cut, which limits its usability for thicker crystals. With LIOB on the other hand, it is challenging to incorporate optical barriers close to the crystal surface. Hence LIOB in the center of the crystal and LA close to the surfaces would be a good combination from a technical point of view.

For the combination of LA and LIOB 3 different cases were simulated: LA at the entrance side of the detector, LA at the exit side of the detector, and LA on both sides, as illustrated in Figure 3, part 5. In all cases reflectors were inserted in the laser ablated regions. Two cases were simulated: smooth ablated surfaces and unpolished ablated surfaces, both with external diffuse reflectors. In all cases the reflection coefficient was set to 0.98, and the barrier width was 0.2 mm to match the dead space of the MPPC array.

2.3 Simulation parameters

2.3.1 LYSO:Ce crystal—In all simulations the simulated crystal material was LYSO:Ce with a refractive index of 1.82 at its wavelength of maximum emission, 420 nm. As in our

previous simulations of LYSO:Ce an optical absorption length of 40 cm was used, and optical scattering within the crystal bulk was neglected [33, 45].

2.3.2 Photodetector array—As our photon counting detector concept is based on one-to-one coupling between crystal pixels and photodetector elements, a simplified version of the photodetector array with the smallest pixel size that we have available in our lab was implemented in the simulations. This array is an 8×8 MPPC array from Hamamatsu with 1×1 mm² active pixel area (S13615–1025N-08), and 1.2 mm pitch. While this pixel size is larger than what we are aiming for in a final design we chose to use this in the present study so that we can also couple our results to experiments moving forward. The array was simulated with a 100 μm thick entrance window with a refractive index of 1.55. Optical photons impinging on the active MPPC area were treated as counted, and photons hitting the dead space were subject to specular reflection with a 30% probability, and absorption with 70% probability. These values were chosen based on our conversations with the manufacturer. It should however be noted that the modeling of the dead space is a source of uncertainty in these simulations as we were not able to obtain a detailed description of its properties. We have simulated a range of reflectivity values for this surface, and based on these we do not expect a significant effect with respect to the conclusions drawn in this paper.

2.3.3 Optical barriers—As in our previous simulation studies [33, 45] the optical barriers were modeled as slabs (50–200 μm wide) with varying refractive index. The interface between the optical barrier and the crystal bulk was modeled with varying roughness. A completely smooth interface was simulated using the POLISH surface model in DETECT2000. To simulate a rough interface the UNIFIED surface model available in DETECT, with 100% specular lobe reflection and a value of the σ_a parameter of 20°, was used. The value of σ_a parameter corresponds to the standard deviation of a Gaussian distribution of surface normal around the nominal surface normal [51]. This approach is commonly used to describe the surface roughness of an unpolished scintillator crystal. The same surface models were used to describe the outer surfaces of the monolithic crystal and the mechanically cut pixels.

2.4 Simulation procedure

For each detector configuration X-ray interactions were simulated at several discrete depths with 250 μm step size in the z direction. For the combinations of LA and LIOB (Section 2.2.3.4) the step size was reduced to 200 μm, in order to have a source location within the ablated regions. At each discrete depth 1000 X-ray events were simulated in a crystal pixel above a central MPPC pixel. At a given depth the event positions were uniformly and randomly distributed across the crystal pixel cross-section. Each event was simulated as an isotropic point source of 800 optical photons. This number was chosen to simulate 70 keV X-rays and is based on the ~30 photons/keV light yield of LYSO:Ce, in combination with a photo detection efficiency (PDE) of the MPPC of ~35%. Hence in the simulations the PDE of the MPPC array was set to 100% as the signal loss in the photoconversion step was accounted for already by the number of generated optical photons. This was done in order to speed up simulations. It should be noted that all references to PDE in this work corresponds

to the efficiency with which optical scintillation photons are converted to photoelectrons by the photodetector, not to the X-ray detection efficiency of the detector.

In the case of multiple crystal pixels per MPPC pixel (Section 2.2.3.3), sources were simulated in representative crystal pixels above one central MPPC pixel, as described in Figure 4. The number of photons collected by each MPPC pixel was recorded, as well as the fraction of photons that were absorbed at surfaces or in the crystal bulk, timed out or escaped from the geometry.

It should be emphasized that these simulations only take into account transport of optical photons, and not the actual interaction of the X-ray photons in the detector. The term *source* is therefore exclusively referring to the source of optical photons, which corresponds to the interaction location of the X-ray photon in the crystal, as opposed to the X-ray source itself.

2.4.1 Extracted performance metrics—For clarity, Table 1 summarizes different metrics discussed in this paper. The ones related to the optical light transport in the scintillator are further described in the following subsections. The metrics derived from the simulation data were calculated as averages over all simulated events.

2.4.1.1 Light Confinement: The light confinement was defined as the number of optical photons collected by the MPPC pixel located directly underneath the source (i.e. X-ray interaction point), divided by the total number of optical photons collected by the whole MPPC array. It should be noted that this convention was used for all pixels in the patterns described in Section 2.2.3.3, even though in these cases there is not one-to-one coupling between crystal pixel and MPPC pixel and hence the confinement is associated with cross-talk between MPPC pixels rather than between crystal pixels..

2.4.1.2 Optical cross-talk: Three different cross-talk metrics were calculated, as described in Figure 5. In all cases the cross-talk is calculated as the sum of the signal in the adjacent pixels divided by the signal in the source pixel. C1 takes into account the 4 nearest neighbors to the MPPC pixel below the source, C2 corresponds to the cross-talk within a box of 8 pixels around the source pixel, and C3 a box of 24.

2.4.1.3 Light collection efficiency: The light collection efficiency (LCE) was recorded for each simulated detector configuration and was defined as the fraction of all optical photons emitted in an event that were collected by the whole MPPC array.

3 Results

3.1 Mechanically pixelated array and monolithic crystal

Table 2 summarizes the results obtained for the mechanically pixelated array and the monolithic crystal. Four cases were simulated: perfect reflectors across the whole pixel, 100 μm missing from the bottom, 100 μm missing from the top, and 100 μm missing from both the top and the bottom of the pixels. For each configuration both polished and unpolished surfaces were studied.

The results show that both confinement and light collection efficiency are higher for the unpolished pixels. The light collection efficiency is drastically reduced when all surfaces are polished (>50% lower, compared to unpolished for geometry **A**), as a consequence of light trapping which leads to high bulk absorption. When some parts of the unpolished pixels are left without reflectors, the light collection efficiency decreases by 3.3%, 7.7% and 10.4% for geometries **B**, **C** and **D** respectively. For the polished case the light collection efficiency is instead increased by 5% for geometry **B**, and 3.1% for geometry **D**, and decreased by 0.7% for geometry **C**.

For unpolished pixels the confinement decreases, as expected, when part of the reflector is missing. Decreases of 3.3%, 3.6% and 6.8% were observed for geometries **B**, **C** and **D**, respectively, showing that missing reflector on one crystal end has similar effect regardless of side. The light confinement for polished pixels has the corresponding behavior as for the light collection efficiency. Geometry **C** results in a slight increase in confinement (0.4%) while **B** and **D** gives decreased confinement by 3.6% and 2.4%, respectively. Missing reflectors on both sides thus results in better performance, from the confinement perspective, compared to when the reflector is only missing from the side that is close to the photodetector. In all cases depth dependence, manifested as larger standard deviations, in both confinement and light collection efficiency is observed when imperfect reflectors are used. Even though light confinement is not really a concept in a monolithic crystal, as no light confining structures are incorporated into the detector, we chose to determine how many photons are collected in the MPPC element closest to the source also for this configuration. In this case the events were distributed over a $1 \times 1 \text{ mm}^2$ cross-section above a central MPPC pixel at each depth. It is observed that the confinement is higher for a polished crystal compared to an unpolished one. Furthermore, one can see that the light collection efficiency is significantly higher in the unpolished crystal. The main reason for this is increased bulk absorption in the polished case, as light tends to be trapped by total internal reflection. A depth dependence of the confinement is also observed mainly in the polished case, which is causing the large standard deviation in the confinement values. The light collection efficiency is however essentially independent of depth.

3.2 Laser-processed detectors

Figure 6 summarizes the results for all types of laser-processed detectors. Details for each pattern category can be found in Sections 3.2.1 to 3.2.4. One general trend across all configurations is that higher confinement but lower light collection efficiency is observed for smooth barrier/crystal interfaces compared to rough interfaces. The lower light collection efficiency in the smooth case is caused by increased bulk absorption due to trapping by total internal reflection. Furthermore, the confinement always decreases with higher barrier RI, as the barrier properties approach those of the crystal bulk (**B**). For smooth interfaces the light collection efficiency tends to decrease with increasing barrier RI, while the opposite behavior is observed for the rough interfaces (**C**). The difference between smooth and rough interfaces is also smaller for higher RI, both in terms of light confinement and light collection efficiency. Regardless of barrier pattern, the confinement in the laser-processed detectors is always lower compared to the mechanically pixelated array. The highest achievable confinement for smooth interfaces is 88.6% observed for the geometry with

ablation on both top and bottom in combination with an RI of 1.0 (**B6**). However, no other configuration (apart from smooth ablation only in the bottom part, see Figure 12) was observed to yield a confinement above 80%. For rough interfaces the highest confinement observed was 65.7% for the central pixel in the 5×5 pattern (**B5**), followed by 64.7% for the triple barriers (**B3**).

One observation is that the confinement tends to increase by adding more optical barrier walls. This is true regardless of barrier RI for rough interfaces, and here the effect is biggest when going from single to double barriers. For smooth interfaces the behavior is somewhat less intuitive, and the higher refractive indices (1.4 and 1.6) are associated with increased confinement for double barriers compared to single barriers. For triple barriers the confinement decreases slightly again, but still remains higher compared to the single barriers. For low refractive indices (1.0 and 1.2) the confinement slightly decreases when moving from single to double barriers, and increases again for triple barriers (**B1–B3**). In general, the confinement effect from adding more barrier walls is more pronounced for the rough interfaces.

For 3×3 and 5×5 crystal pixels per MPPC pixel (**A4, A5**), the results are shown for the central crystal pixel, which has the highest confinement across the array. It can be seen that for the rough interface the confinement is increased compared to the single barrier while for the polished case it is decreased (**B4, B5**). For this configuration the confinement is less dependent on the interface roughness compared to the one-to-one match case. The light collection efficiency is increased in both cases (**C4, C5**).

Finally, it can be seen that also a combination of LIOB and laser ablation can be used to increase confinement beyond that of the simple single barrier case (**B6**). In this figure the case with ablation both in the top and bottom part of the detector is shown, and the ablated region is defined as smooth with an external diffuse reflector. While the confinement is only slightly increased by the ablation for rough barrier/crystal interfaces, the effect is more drastic for smooth interfaces. The LCE is increased for rough interfaces but decreased for smooth interfaces (**C6**) compared to LIOB all the way through the crystal. The light collection efficiency is also more uniform across the RI range compared to when LIOB is used throughout the crystal.

3.2.1 Single barrier—Figure 7 shows the confinement, light collection efficiency and cross-talk for 5 varieties of the single barrier wall pattern. The 5 configurations differ in the optical barrier wall thickness (d_{OB}), as well as the width of the MPPC dead space (d_{DS}). For each configuration the barrier RI and the barrier/crystal interface roughness is varied. As the values obtained depend heavily on the interface roughness we have chosen to divide those two cases to be able to visualize more subtle differences within each subgroup.

The results show that the highest confinement is achieved for $d_{OB}=d_{DS}=200\text{ }\mu\text{m}$ (blue). This is true regardless of barrier RI and barrier/crystal interface roughness, and 79.7% confinement can be achieved in the ideal scenario of RI=1.0 and a perfectly smooth interface. The corresponding number for a rough interface is 50.3%. As expected, the confinement decreases from these values for increasing barrier RI. It is further observed that

for smooth interfaces the confinement depends on d_{DS} , with lower confinement for smaller dead space. The confinement appears independent of d_{OB} , as the blue ($d_{OB}=d_{DS}=0.2$ mm) and red ($d_{OB}=0.05$ mm and $d_{DS}=0.2$ mm) curves are very similar. For rough interfaces on the other hand, the confinement depends on d_{OB} , with higher confinement for wider barriers, but in this case there is no apparent dependence on d_{DS} .

The light collection efficiency is higher for rough interfaces compared to smooth interfaces, with a maximum of 94.8% for $RI=1.0$, $d_{DS}=0.025$ and $d_{OB}=0.05$ mm (purple). For smooth interfaces the highest light collection efficiency is 72.9% for $RI=1.4$, $d_{DS}=0.025$ and $d_{OB}=0.05$ mm. In both cases the light collection efficiency decreases with increasing dead space. For the widest dead space ($d_{DS}=0.2$ mm) the confinement is higher for $d_{OB}=d_{DS}$ compared to when $d_{OB}<d_{DS}$. Finally, for smooth interfaces the light collection efficiency tends to increase with increasing barrier RI , while the opposite behavior is observed for rough interfaces.

The cross-talk values show the same trends in C1, C2 and C3 for both smooth and rough interfaces. Consistently with the confinement values the cross-talk is higher for rough interfaces compared to smooth ones. For smooth interfaces one can see a difference (~40% for $RI=1.0$) between the red and blue curves in C1, which was not apparent in the confinement values. This difference is reduced to 30% for C2 and 13% for C3. For rough interfaces there is a small dependence on d_{DS} , visible mainly in C1, which was not present in the confinement.

Across all metrics, the curves are flatter for the rough interfaces, meaning a weaker dependence on barrier RI compared to smooth interfaces. It should be noted that in these simulations the MPPC pitch and overall detector dimensions were kept constant, meaning the active MPPC area was effectively increased when decreasing the dead space. We have also performed simulations where the active area was kept constant and decreasing the dead space decreased the overall detector size. These simulations showed the same trends in the results as the ones presented here.

3.2.2 Multiple barriers—Figure 8 shows a comparison between single, double and triple barriers, where the double and triple barrier line spacing is chosen such that the total barrier thickness (walls + spacing) matches the MPPC dead space of 0.2 mm. Two variations of the single barrier pattern are shown: 1) 0.2 mm barrier width matching the MPPC dead space and 2) 0.05 mm barriers, which is equal to the individual barrier walls in the double and triple barrier patterns. It can be seen that for a smooth interface there is no gain in confinement by adding multiple walls. For rough interfaces there is a significant confinement increase from single to double barriers and a smaller additional gain between double and triple barriers. Double barriers results in 18–24% increased confinement compared to single 0.2 mm barriers. The increase is higher for lower RI values. For triple barriers the confinement increases by ~28% from single barriers regardless of barrier RI . In terms of LCE there is no significant difference when comparing double or triple barriers to the single 0.2 mm barrier pattern for smooth interfaces. For rough interfaces on the other hand, the LCE for both double and triple barriers is similar to the 0.05 mm single barrier pattern.

Figure 9 shows how the results for double and triple barriers vary with the spacing between the optical barrier walls. In all these simulations the thickness of a single optical barrier wall is kept constant at 0.05 mm. For double barriers with smooth interfaces the confinement decreases with decreasing line spacing for the lower RI values. For higher RI, as well as for the rough interfaces (regardless of RI) the confinement is essentially independent of the line spacing. For triple barriers the same trends, although less pronounced, are observed for smooth interfaces. For rough interfaces the confinement is slightly lower for the smallest line spacing compared to all others. The light collection efficiency increases with increasing line spacing in all cases. This trend is slightly stronger for the double barriers compared to the triple barriers. The cross-talk is almost independent of line spacing for smooth interfaces for both double and triple barriers, except for C3 that shows slightly higher cross-talk for larger line spacing for the lower RI values. Double barriers with rough interfaces show higher cross-talk for the largest line spacing compared to all others. For triple barriers with rough interfaces the largest line spacing results in slightly higher C1 for large RI, and the smallest line spacing has elevated C2 and C3 for low RI values.

3.2.3 Multiple pixels per MPPC pixel—Figure 10 shows the results obtained for the geometry with 3×3 crystal pixels per MPPC pixel, and Figure 11 the corresponding results for 5×5 crystal pixels per MPPC pixel.

As expected, the confinement decreases in both cases when the crystal source pixel is located closer to the MPPC pixel edge, regardless of interface roughness and barrier RI. Our definition of confinement represents the amount of light collected in the MPPC pixel directly underneath the source pixel, which for this barrier pattern should not be confused with the traditional confinement within a crystal pixel. In this configuration one can think of the groups of pixels on top of a given MPPC pixel as a macro pixel containing 3×3 or 5×5 micro pixels. In this context we study the confinement in the macro pixel as a function of source placement in the micro pixels. For the 3×3 pattern the confinement is 21–25% lower in the corner pixel compared to the central pixel for smooth interfaces. The corresponding numbers for rough interfaces are 27–29%. The 5×5 pattern has a larger spread among the pixels with the corresponding numbers of 41–43% and 44–46% for smooth and rough interfaces respectively. In both cases the central pixel has the highest confinement, and for smooth interfaces the confinement in this pixel is comparable between the 3×3 and 5×5 patterns (<2% difference across the RI range). For rough interfaces the differences are larger with 7–13% higher confinement in the central pixel for the 5×5 pattern compared to the 3×3 pattern. Further, it can be observed that for the 5×5 pattern all pixels (1, 2 and 4) that are not in contact with the MPPC dead space have very similar confinement values. For the smooth interface these 3 pixels are not distinguishable while for rough interfaces, there is a small decrease in confinement as the source moves closer to the corner. The light collection efficiency shows the same dependence on source location as the confinement, with reduced light collection efficiency close to the MPPC pixel edge and corner due to overlap with the dead space. The trends in the cross-talk values are consistent for C1, C2 and C3, and the overall behavior of the detector is less dependent on surface roughness for the 5×5 case compared to the 3×3 case.

3.2.4 Combination of LIOB and Laser Ablation—The final approach studied in this paper is a combination of LA and LIOB as a mean to increase the light confinement. Figure 12 shows the results for this configuration, where the roughness of the ablated cut is varied in addition to the optical barrier properties. One trend observed in all of the configurations containing ablation is larger error bars in the confinement numbers compared to the all-way LIOB pattern. This is due to increased depth dependence caused by non-uniform properties throughout the crystal thickness. The depth dependence is higher for higher barrier RI, as the light propagation will approach that in a monolithic crystal.

For rough interfaces the confinement is essentially independent of the characteristics of the ablated region, and always similar to the LIOB only configuration. For smooth interfaces on the other hand, the behavior is highly dependent on the properties of the ablated surface. A rough ablated surface results in lower confinement than both smooth ablation and the LIOB only pattern. Here the confinement is highest for LA in the top part of the crystal, and lowest for LA on both sides. The latter is only marginally lower compared to LA only in the bottom part.

For smooth ablation the behavior is somewhat inverted. The highest confinement is achieved for ablation on both sides and is very closely followed by LA in the bottom part only. LA in only the top part yields significantly lower confinement, on a similar level as the LIOB only pattern. In this configuration, LA in the bottom part of the crystal introduces a kink in the confinement at RI=1.2. We have simulated adjacent RI values in this region and the curve is continuous with a local minimum around this value.

The light collection efficiency for rough interfaces is higher for LA on the bottom or both sides compared to LA on the top side. The results are independent on the properties of the ablated region. For smooth interfaces the light collection efficiency is higher for rough ablation compared to smooth, and as for the confinement the efficiency is dominated by the ablation in the bottom part for smooth ablation and by ablation in the top part for rough ablation. The cross-talk is independent of LA characteristics for the rough interfaces, and higher for rough ablation compared to smooth for smooth barrier/crystal interfaces.

4 Discussion and conclusions

We are investigating the feasibility of a scintillator-based PCD (ScPCD) for CT, which could constitute a cost-effective alternative to semiconductor-based PCDs and open up new avenues for practical and low-dose whole-body CT imaging. Historically the PCD development for CT has been focused on semiconductor detectors, while scintillators are the mainstay detector type for photon counting in other medical imaging modalities such as PET and SPECT.

One major challenge for any PCD to be used in CT is the high X-ray flux, which requires a detector solution able to cope with extremely high count rates if to be used in a clinical setting. This has historically been a hurdle for ScPCDs due to the lack of a feasible way of fabricating the finely pixelated detector arrays needed to reduce the count rate burden per

electronic channel. Following new potentially enabling fabrication technologies that have emerged in recent years we are now revisiting the ScPCD for CT.

In this paper we are studying the light transport in scintillator arrays fabricated using the so-called Laser Induced Optical Barrier (LIOB) technique, as well as a combination of the LIOB and Laser Ablation (LA) techniques on 2 mm thick LYSO:Ce detectors, and compare them to mechanically pixelated arrays. The detector level performance characterized by light confinement and light collection efficiency are key components of such a detector when used for spectral CT, as it will determine both the spatial and energy resolutions and also impact noise and count rate capabilities of the system. Future work entails coupling the simulations to experiments, as well as evaluation of the rest of the signal chain in a complete scintillator-based PCD, including photodetector and readout electronics.

It should be noted, that some issues present in semiconductor detectors, such as pileup and cross-talk, would most likely still be issues for ScPCDs, especially at high count rates. We do however believe that the benefits of high stopping power and low cost motivates exploring scintillators for this application, as it could be an alternative to semiconductors and facilitate the scaling of spectral CT to clinical use.

The conceptual detector outlined here is different from the scintillator based EIDs used in conventional CT, in that EIDs are typically based on Cadmium Tungstate (CWO) which has comparable stopping power to LYSO:Ce, but much longer decay time, making them unsuitable for operation in pulse mode given the high count rates in clinical CT. While there has been previous efforts in developing microcolumnar scintillator detectors suitable for photon counting CT [52, 53], these are associated with limitations in count rate and achievable detector thickness which results in low dose efficiency. Furthermore, these microcolumnar detectors were based on CsI:Tl, which similarly to CWO has a long decay time [54]. Light confinement in microcolumnar structures is also limited to less than ~30% depending on the material and crystal thickness. This can be one main reason that this structure type has not been explored much for photon counting CT applications.

The present study entails light transport simulations using the Monte Carlo code DETECT2000. A variety of laser-processed detector configurations have been implemented, as well as the industry standard being a mechanically pixelated array. All detector configurations are based on simple pixel-like structures, being the most straightforward approach for detector segmentation. Per each configuration the roughness of the barrier/crystal interface, as well as the barrier RI were varied, given that these properties can be controlled to some extent by tuning laser parameters during processing. Noteworthy that all the simulations reported here are based on using $1 \times 1 \text{ mm}^2$ photodetector elements with 1.2 mm pitch to match with the smallest commercially available MPPCs.

The most basic laser-processed detector configuration studied in this work is one wall of optical barriers separating each pixel-like volume, and one-to-one coupling between the crystal pixels and MPPC pixels. In this configuration we have shown that a confinement of ~80% is achievable for RI=1.0 and a smooth barrier/crystal interface (see Figure 7). For a rough interface the confinement is however significantly lower (~50% for RI=1.0), and the

confinement decreases with increasing barrier RI for both interface types. This trend of decreasing confinement for higher RI and rough interfaces has been observed across all detector configurations in this study. It is further observed that in general there is a trade-off between light confinement and light collection efficiency, in that a higher confinement is usually accompanied by lower light collection efficiency. The degree of overlap between the optical barrier wall and the MPPC dead space affects the light transport characteristics and it was found that for rough interfaces the confinement is mainly dependent on the width of the optical barrier wall (higher confinement for thicker wall), while for smooth interfaces the dependence is mainly related to the width of the dead space (higher confinement for wider dead space). It should be noted that a thick optical barrier wall is not necessarily a negative point in the envisaged application, as anti-scatter grids are common in CT. Therefore, an optical barrier wall which is thinner than the anti-scatter grid septa would not decrease the overall dose efficiency. Furthermore, in previous work no loss in detection efficiency was observed by presence of optical barriers compared to unmodified crystal, suggesting that the optical barriers may not be completely dead with respect to X-ray interactions [34].

In order to investigate the possibility of increasing the light confinement further beyond the single barrier walls three additional approaches were studied: 1) Having multiple barrier walls separating each pixel like structure. 2) Having multiple equally sized crystal pixels per MPPC pixel resulting in a structure that combines long and short-range confinement. 3) Combining the LIOB technique with laser ablation in the top and/or bottom part of the crystal.

For the first approach the simulations showed that it is indeed possible to increase the confinement by up to 24% by switching from single barriers to double barriers (see Figure 8). Adding additional barriers beyond this can increase confinement further, but only marginally (28% increase for triple barriers compared to single barrier). This increase is however only observed for rough interfaces, and the performance for smooth interfaces is essentially unchanged when increasing the number of barrier walls. The spacing between the barriers, affecting the degree of overlap between the total barrier wall thickness and the MPPC dead space, impacts the confinement by higher confinement with small spacing for smooth interfaces. For rough interfaces the spacing does not have a significant impact (see Figure 9).

Having multiple crystal pixels per MPPC pixel results in increased confinement in the central pixel for rough interfaces, but is associated with a decreased confinement for smooth interfaces (see Figure 6). For this configuration there is a variation in confinement, light collection efficiency and cross-talk depending on in which crystal pixel the interaction takes place (see Figure 10 and Figure 11). This feature may be exploited to increase the spatial resolution beyond the MPPC pixel size by employing positioning algorithms based on light sharing such as simple Anger logic or more sophisticated statistical methods like Maximum Likelihood. While these approaches are routinely used for PET and SPECT applications, their implementation in CT requires high speed detectors due to the inherent high count rate (up to $10^8/\text{mm}^2/\text{s}$). Similar concepts of long and short range confinement have previously been explored in pixelated microcolumnar detectors [29, 55]. It is further observed that

increased number of crystal pixels per MPPC pixel results in a lower dependence on the interface roughness.

The final approach is the combination of LIOB and laser ablation (LA). Such combination would be straightforward to achieve experimentally given that the same laser system can be used for both techniques, and the combination would solve inherent limitations of each technique (difficulties to process close to surfaces for LIOB, and difficulties to achieve uniform cuts for thicker crystals for LA). Intuitively, the introduction of cuts filled with reflective material should increase the confinement within crystal pixels, as the possibility for photons to travel through the pixel wall is essentially eliminated in this case. However, as seen in Figure 12 this configuration yields a complicated behavior. The first observation is that the performance is strongly dependent on both the roughness of the ablated cut, and the roughness of the barrier/crystal interface. For rough barrier/crystal interfaces the confinement is essentially unchanged by adding laser ablation, and the light collection efficiency is unchanged for LA in the top part of the crystal but increased for LA in the bottom part (meaning close to the photodetector). For smooth interfaces the confinement is increased by adding smooth ablated cuts in the bottom part of the crystal, unchanged by smooth cuts in the top part, and decreased by rough cuts, compared to the LIOB only configuration. The light collection efficiency has the opposite behavior with decrease for smooth cuts, and increase for rough cuts.

A general trend across all simulated detector configurations is that there is a trade-off between the light confinement and the light collection efficiency. Ideally, one would want 100% LCE and 100% confinement. Similar to semiconductor-based PCD, where 0% charge sharing and 100% charge collection within the pixel is considered ideal. While achieving these values, especially 0% charge sharing, is not practical, various techniques have been explored to mitigate this issue such as summing charge across neighboring pixels to the one with largest signal. In fact, similar techniques can be used in ScPCD to further increase light collection and hence energy resolution.

The light collection efficiencies in laser-processed detectors were found comparable to that in mechanically pixelated arrays. Rough interfaces resulted in higher LCE compared to smooth interfaces, analogous to higher LCE for unpolished crystals compared to polished crystals for the mechanically pixelated and monolithic detectors. One major reason for this is the breaking of symmetry incurred by the diffuse surfaces that result in less trapping of light.

As mentioned earlier we chose 1 mm photodetector pixel size with 1.2 mm pitch since MPPCs with this size are the smallest commercially available devices. While this pixel size is larger compared to what we envisage in a final design, it was chosen to enable coupling of the simulations to experiments moving forward. Table 3 presents preliminary simulation results comparing the light channeling capabilities of 1 mm and 0.5 mm scintillator pixels in order to estimate the effect that reduced pixel size may have on the light transport. It is apparent that the choice of photodetector for the optical photoconversion will greatly impact the results, which is why in these simulations the light transport is decoupled from the conversion of optical photons to electrical signal, due to the absence of a commercially

available photodetector with 0.5 mm pixel size or smaller. In this regard the amount of light reaching the exit surface of each crystal pixel is studied as a function of barrier properties and crystal pixel size. It should be noted that only geometrical effects are considered in these simulations with no photon absorption applied. As reported in the table the cross-talk is increasing with decreased pixel size for rough barrier/crystal interfaces, but decreases for smooth interfaces. The reason for this counterintuitive behavior for smooth interfaces is the geometric factors on a microscopic level in that despite a slight decrease in light channeling, neighboring pixels will have smaller signals as well due to smaller dimension compared with $1 \times 1 \text{ mm}^2$ pixels. Therefore, the reduction of light collected in neighboring pixels is larger compared with the reduction of light exiting the intended pixel, resulting in a reduced overall cross-talk.

It is noteworthy that the final detector design and photodetector type are not studied in this paper, and therefore it is not straightforward to predict the ultimate performance of a smaller pixel system based on the simulations reported here. However, we believe that the trends observed for the 1 mm pixels, both in terms of barrier properties and barrier patterns, should hold also for smaller pixel size. Some loss in confinement and LCE can be expected when reducing the pixel size, however our conceptual design incorporates ASICs with built in photodiodes, which are well known to have significantly higher quantum efficiency compared to MPPCs and the potential light loss may hence be compensated for. It should further be noted that increased cross-talk for smaller scintillator pixels is analogous to increased charge sharing for semiconductors (a. k. a. the “small pixel effect”).

It should be noted, that even though we have identified ways to increase the light confinement in laser-processed detectors, it is always lower compared to an *ideal* mechanically cut array. However, it is apparent that LIOB offers a high level of flexibility that mechanical pixelation does not have. While the 1 mm pixels studied in this paper may be fabricated using mechanical pixelation, it is extremely difficult to obtain pixels with smaller (sub-mm) cross-section such as 0.2 mm, needed to cope with the high count rates in CT. The LIOB technique is a promising approach to achieve such fine pixel pitch [56], and hence might be the enabling technology needed for scintillators to be feasible as PCDs in CT.

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Figure 1. Transmission as a function of detector thickness for 70 and 140 keV X-rays. Shown is data for a few detector materials relevant for CT. Absorption data to generate the plots is taken from [40].

Figure 2.
Schematic drawing of the conceptual design of the ScPCD.

Figure 3.

Schematic drawings of the laser-processed detector configurations. **1:** Simulated detector geometries with single optical barrier walls between each pixel like volume. **1.a)** $d_{OB}=d_{DS}$, **1.b)** $d_{OB}<d_{DS}$, **1.c)** $d_{OB}>d_{DS}$. **2 and 3:** Double and triple barrier walls between each pixel like volume. **2 a)** and **3.a)** $d_{TOT}=d_{DS}$, **2.b)** and **3.b)** $d_{TOT}=d_{DS}+d_{OB}$, **2.c)** and **3.c)** $d_{TOT}=d_{DS}+2d_{OB}$, **2.d)** and **3.d)** $d_{TOT}=d_{DS}+3d_{OB}$. **4:** of 3×3 (**4.a)** and 5×5 (**4.b)** crystal pixels per MPPC pixel. Here both side and top views of the geometries. **5:** Laser-processed detectors with a combination of LIOB and LA. **5.a)** LA in the bottom part of the detector. **5.b)** LA in the top part of the detector. **5.c)** LA in both the top and bottom part of the detector. Note that for purposes of clarity all drawings show fewer pixels than in the simulated geometries.

Figure 4.

Schematic illustration of source placement during simulations. **A:** Optical photons were generated in crystal pixels above one central MPPC pixel, shown in black. **B:** Position of crystal pixels above one MPPC pixel for the case of 3×3 crystal pixels per MPPC pixel. Numbers indicates crystal pixels where events were simulated. **C:** As **B** but for 5×5 crystal pixels per MPPC pixel.

Figure 5.
Illustration of how the cross-talk metrics were calculated. The figures highlight which pixel signals are taken into account in the calculation of the cross-talk. The black pixel corresponds to the MPPC pixel located directly under the source.

Figure 6.

Summary of the results for the different laser-processed detector configurations. 1: 0.2 mm wide single OB wall coupled one-to-one with MPPC array coupling. Details of varieties of this configuration can be found in Figure 7. 2: Double wall of OB (details in Figure 9 a). 3: Triple wall of OB (details in Figure 9 b). 4: 3x3 crystal pixels per MPPC pixel (details in Figure 10). 5: 5x5 crystal pixels per MPPC pixel (details in Figure 11). 6: Combination of LIOB and Laser Ablation (LA) (details in Figure 12).

Figure 7. Summary of the results obtained with the single barrier wall pattern. All results are shown as a function of barrier RI and different subplots show the results for rough and smooth interfaces respectively. All values are averages over all crystal depths, and the error bars correspond to the standard deviation across all events.

Figure 8. Comparison between single, double and triple barriers. The figure shows confinement and light collection efficiency for smooth and rough interfaces respectively.

Figure 9.
Confinement, light collection efficiency and cross-talk for a) double barriers and b) triple barriers.

Figure 10. Confinement, light collection efficiency and cross-talk for 3x3 crystal pixels per MPPC pixel.

Figure 11. Confinement, light collection efficiency and cross-talk for 5x5 crystal pixels per MPPC pixel

Figure 12.

Confinement, light collection efficiency and cross-talk for a combination of optical barriers and laser ablation, compared to the LIOB only pattern with single barrier walls (0.2 mm thick) separating each crystal pixel. In all cases the ablated cut is 0.2 mm. Solid lines correspond to a smooth ablated surface, and dashed lines to a rough ($\sigma_a=20^\circ$) surface

Table 1.

Summary of detector properties of interest in this paper.

Property	Abbreviation	Definition
Light Confinement	Conf.	# of optical photons collected by the MPPC pixel underneath the X-ray interaction point / # of optical photons collected by the complete MPPC array.
Optical Cross-talk	C1, C2, C3	# of optical photons collected by adjacent MPPC pixels / # of photons collected by the MPPC pixel underneath X-ray interaction point. See Figure 5 for details on the three varieties.
Light Collection Efficiency	LCE	# of optical photons collected by the whole MPPC array / # of optical photons emitted at the X-ray interaction point.
X-ray Detection Efficiency		# of X-rays detected / # of X-rays impinging on the detector.

Table 2.

Summary of simulation results for the mechanically pixelated array and the monolithic crystal.

Conf.=Confinement, C1–C3=cross-talk and LCE=Light collection efficiency, as described in Section 2.4.1.

Cross-talk values are omitted for the monolithic crystal. The given values are averages over all depths and the uncertainties correspond to the one σ variation across all events.

Geometry	Surfaces	1: Conf. (%)	2: C1 (%)	3: C2 (%)	4: C3 (%)	5: LCE (%)
A: Complete reflector	Polished	90.74 $\pm$ 1.81	8.24 $\pm$ 1.95	9.53 $\pm$ 2.14	10.15 $\pm$ 2.22	41.84 $\pm$ 1.91
	Unpolished	95.98 $\pm$ 0.96	3.58 $\pm$ 0.94	4.095 $\pm$ 1.03	4.18 $\pm$ 1.05	84.87 $\pm$ 1.49
B: Reflector missing on bottom	Polished	87.16 $\pm$ 2.14	11.18 $\pm$ 2.30	13.14 $\pm$ 2.57	14.54 $\pm$ 2.83	43.93 $\pm$ 2.00
	Unpolished	92.78 $\pm$ 2.68	6.36 $\pm$ 2.52	7.35 $\pm$ 2.95	7.85 $\pm$ 3.26	82.00 $\pm$ 2.30
C: Reflector missing on top	Polished	91.07 $\pm$ 1.77	7.49 $\pm$ 1.86	8.98 $\pm$ 2.07	9.69 $\pm$ 2.16	41.55 $\pm$ 1.89
	Unpolished	92.52 $\pm$ 1.48	6.57 $\pm$ 1.46	7.60 $\pm$ 1.64	8.09 $\pm$ 1.76	78.37 $\pm$ 2.29
D: Reflector missing on both ends	Polished	88.44 $\pm$ 2.40	9.74 $\pm$ 2.53	11.62 $\pm$ 2.82	12.87 $\pm$ 3.08	43.14 $\pm$ 2.11
	Unpolished	89.45 $\pm$ 2.51	9.26 $\pm$ 2.49	10.84 $\pm$ 2.92	11.84 $\pm$ 3.26	76.09 $\pm$ 2.27
E: Monolithic	Polished	19.7 $\pm$ 10.2				38.08 $\pm$ 1.85
	Unpolished	9.75 $\pm$ 5.31				74.72 $\pm$ 1.66

Table 3.

Simulated cross-talk as a function of scintillator pixel size, without coupling to a photodetector. All simulations were performed for 2 mm thick LYSO, and the optical barriers were simulated as 0.05 mm thick slabs. As in the rest of this paper a rough interface corresponds to $\sigma_a=20^\circ$. For the 1 mm pixels an array of 10×10 pixels is simulated, and for the 0.5 mm pixels an array of 20×20 pixels in order to keep the total detector size constant. A point source of 100k photons was simulated at 7 depths (0.25 mm separation in z) in a central crystal pixel. The presented values are averages over all depths. C1 is defined as the sum of the signal in 4 nearest neighbors divided by the central pixel, C2 takes into account the 8 nearest neighbors, and C3 the 25 nearest neighbors, analogous to the metrics defined in Section 2.4.1.2. The reported uncertainties correspond to the standard deviation of the results across all simulated depths. Note that the cross-talk values are reported in percentage. 100% cross-talk means that 50% of the light exits the source pixel and the other 50% are collected by the neighboring pixels.

	C1 (%)		C2 (%)		C3 (%)	
	1 mm	0.5 mm	1 mm	0.5 mm	1 mm	0.5 mm
RI=1.0, smooth	8.6 ± 2.1	4.0 ± 2.1	9.6 ± 2.0	4.9 ± 2.2	18.3 ± 1.6	8.6 ± 2.5
RI=1.0, rough	37.0 ± 3.3	49.8 ± 5.6	45.4 ± 4.3	66.4 ± 8.4	66.8 ± 8.1	91.3 ± 12.3