High Z and Medium Z Scintillators in Ultra High Resolution Small Animal PET

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Abstract—As small animal PET scanners are continuously improving in their performances, one is lead to the question of how far can spatial resolution go. In this paper we address the limiting effects to spatial resolution and whether the photoelectric interaction, and therefore high Z materials, outperform medium Z scintillators. In particular, with a Monte Carlo simulation, we compare the ultimate performances, in spatial resolution, of three scintillators: BGO, NaI(Tl) and YAP:Ce. BGO is the PET scintillator which has the highest photofraction whereas YAP:Ce has the lowest. NaI(Tl), instead is a relatively high Z but low density scintillator. There are three principle contributions to the degradation of spatial resolution: multiple Compton scattering electron range after a gamma interaction and K-shell fluorescence emission. We present the results of simulations of crystals with different thicknesses, with and without K-shell fluorescence emission and electron transport. We conclude that the effect of multiple scattering, electron range and fluorescence emission to the spatial resolution are smaller for low Z, high density materials like YAP:Ce. The fraction of misplaced events, defined here as \( F = \frac{N_{\text{Wrong}}}{N_{\text{Tot}}} \), is \( F_{0.1\text{mm}} = 52\% \) for BGO in the case of 0.5 mm binning, increasing to \( F_{0.1\text{mm}} = 80\% \) for the 0.1 mm binning. In the case of YAP:Ce, the scatter fractions are respectively \( F_{0.1\text{mm}} = 27\% \) and \( F_{0.1\text{mm}} = 44\% \). We conclude that for ultra high resolution PET detectors, medium Z scintillators, such as YAP:Ce, may outperform high Z materials.

I. INTRODUCTION

In recent years, there has been considerable research in the use of small animal PET scanners, especially for high Z materials, to improve the performance of future PET scanners. An important example is LuAP:Ce with its high Z, high density, fast decay time and relatively high light yield. It is well known, though, that all high Z materials, in any case, have a photofraction below 50% at 511 keV. This implies that events under the full energy peak will have a large contribution from multiple Compton scattering. These events are usually chosen as ‘best’ events. In low Z scintillators, by selecting only Compton events, a high fraction of these (>65%) will be single interactions. This is more than any photofraction of known scintillators.

Two other factors also must be considered: electron range after an interaction and K-shell fluorescence emission. In Table I are reported the \( K_{\alpha} \) and \( K_{\beta} \) X-ray energies, their gamma mean free path (GMFP) and the average electron range after an interaction. The probability of K-shell fluorescence emission after a photoelectric absorption is very high (>90%) for elements with high Z, and, the higher the atomic number of the material, the higher the K fluorescence X-ray energy will be. Furthermore the energy of fluorescent X-rays is just below the K-edge where absorption is at a local minimum. In BGO scintillator, the GMFP of a K\(_{\beta}\) fluorescence is just under 1 mm whereas in YAP:Ce it is only \( \approx 150\mu m \).

After a photoelectric interaction the secondary electron will have an energy somewhere above 440 keV. These will travel just under 200 µm in BGO and LSO whereas for medium Z scintillators where Compton interactions are chosen, these will travel on average below 100 µm.

All of these facts will produce multiple events in the detector, limiting, therefore, the ultimate precision in the position determination of an event.

<table>
<thead>
<tr>
<th>Material</th>
<th>NaI(Tl)</th>
<th>BGO</th>
<th>LSO</th>
<th>YAP:Ce</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density g/cm(^3)</td>
<td>3.76</td>
<td>7.13</td>
<td>7.4</td>
<td>5.37</td>
</tr>
<tr>
<td>Light yield %NaI(Tl)</td>
<td>100</td>
<td>15</td>
<td>75</td>
<td>55</td>
</tr>
<tr>
<td>Atomic numbers</td>
<td>11.53</td>
<td>83.32</td>
<td>48</td>
<td>71.32</td>
</tr>
<tr>
<td>Decay time (ns)</td>
<td>230</td>
<td>300</td>
<td>40</td>
<td>27</td>
</tr>
<tr>
<td>Photoelectric fraction @ 511 keV</td>
<td>18%</td>
<td>44%</td>
<td>34%</td>
<td>4.4%</td>
</tr>
<tr>
<td>K fluorescence (keV)</td>
<td>28.6</td>
<td>77.1</td>
<td>87.34</td>
<td>54.1</td>
</tr>
<tr>
<td>fluorescence GMFP (mm)</td>
<td>0.32</td>
<td>0.68</td>
<td>0.93</td>
<td>0.56</td>
</tr>
<tr>
<td>electron range @ ( E_{\text{dep}} ) (mm)</td>
<td>0.43</td>
<td>0.18</td>
<td>0.19</td>
<td>0.07</td>
</tr>
<tr>
<td>GMFP @ 511keV (cm)</td>
<td>2.85</td>
<td>1.04</td>
<td>1.15</td>
<td>2.18</td>
</tr>
</tbody>
</table>

Medium Z scintillators, which at 511 keV produce principally Compton scattering, may be the possible alternative for precision position determination. An example...
of such a scintillator is YAP:Ce which has only a 4% photofraction, but relatively high density: 5.37 g/cm². In fact the YAP-(S)PET scanner, developed at the University of Ferrara[1], has experimentally shown that by choosing Compton events, and discarding full energy events, the spatial resolution of the system improves significantly[2].

The spatial resolution of small animal scanners is continually improving, and methods of deconvolving positron range effects in reconstruction are also underway. One can imagine that detectors with a spatial resolution below 0.5 mm will soon be developed.

We present here the results from simulations of three crystals, BGO, NaI(Tl) and YAP:Ce, where we have varied the thicknesses of the crystals and where we have artificially turned off the K-fluorescence emission and electron transport. We chose BGO, YAP:Ce and NaI(Tl) because they are the PET scintillators with the highest and lowest atomic numbers, (Z), and NaI(Tl) has a relatively high Z but low density.

II. METHOD

The geometry we simulated is that of the YAP-(S)PET scanner[1,2] with two pairs of opposing scintillator detectors. Each detector has a surface area of 4x4 cm² and the detectors are 15 cm apart.

In the simulations 2 back-to-back 511 keV gammas were always generated and the performance of one of the two detector heads was considered. In energy selection, both opposing detectors were thresholded: an energy threshold of 350 keV implies that both opposing detectors must have a signal above 350 keV. The profiles which will be presented therefore represent coincidence counts.

First, we simulated an ideal detector configuration, using the EGSnrc Monte Carlo code, where a pencil beam of 511 keV gamma rays are incident perpendicular to a slab of scintillator. The crystals have a 4x4 cm² surface and two thicknesses were chosen: 0.2 to 1.0 times the gamma mean free path (GMFP) at 511 keV. This was done to understand the contribution of multiple scattering, K-fluorescence and electron transport to the degradation of spatial resolution.

Secondly, we simulated the case of a uniformly illuminated pixel with gammas incident at 90° to the surface of the scintillator and determined the profiles of the reconstructed coordinates. To determine the profiles, in this case, the coordinate of the reconstructed event was calculated as the average position with the energy deposited at each point as the weighing parameter. In practice though this is not feasible and was done only to see how well each scintillator could reproduce the box shaped profile which was expected.

To be more realistic, in both situations, the position of a reconstructed event was determined following the scheme of a position sensitive readout system based on a resistive charge divider. It is known that the light distribution exiting a crystal with high aspect ratio is uniform, independently of the scintillation position within a pixel. A center of mass readout system, as is a resistive charge divider, can therefore only determine the average position of a uniform distribution which is its center. A typical image of a matrix scintillator as seen by a position sensitive photomultiplier is shown in Figure 1.

![Figure 1: Image of a CsI(Tl) scintillator matrix as seen by a position sensitive photomultiplier tube based on a charge divider readout. Only the position of the center of each pixel can be determined independently of the scintillation position within a pixel.](image)

The X and Y coordinates of an event are therefore calculated using the expressions

$$ X = \frac{\sum_{i=1}^{n} E_i x_i}{\sum_{i=1}^{n} E_i} ; \quad Y = \frac{\sum_{i=1}^{n} E_i y_i}{\sum_{i=1}^{n} E_i} $$

where $E_i$ is the energy deposited in a given pixel whereas $x_i$ and $y_i$ are the coordinates of the centers of the $i$-th pixel.

In the simulations two different energy selections were performed for each scintillator. One, common to all scintillators, was with a lower energy threshold of 50 keV. In the case of BGO and NaI(Tl) the second selection was a lower energy threshold of 350 keV as is commonly done with these scintillators in PET applications whereas for YAP:Ce an upper energy threshold was applied at 400 keV to eliminate full energy absorption events.

Light transport and collection was not considered at this stage but we assumed that each pixel of the matrix could be identified in the image.

A thickness of 0.2 GMFP at 511 keV was chosen to reduce multiple Compton scattering and to see the contribution of K-shell fluorescence emission and electron range. In this configuration, we simulated the system with both K-shell emission and electron transport turned on and turned off.

Three different pixel sizes were simulated: 0.5 mm, 0.2 mm and 0.1 mm. Each profile was binned using the same bin width as the simulated crystal pixel.

A. Fraction of misplaced events and signal to noise ratio

In the first simulations where only the center of each pixel was illuminated, the parameter we have chosen to qualify a scintillator was the fraction of misplaced events $F = \frac{N_{Wrong}}{N_{Tot}}$.

Given, instead, a uniformly illuminated pixel within a matrix, and given the reconstructed coordinates using expression (1), a certain number of events, $N_{right}$, will
populate the correct image pixel corresponding to the illuminated pixel, whereas a certain number, $N_{\text{wrong}}$, will be reconstructed outside. We will define a signal to noise ratio $S/N$ as

$$
\frac{S}{N} = \frac{N_{\text{right}}}{N_{\text{wrong}}}
$$

This is justified by the fact that if the whole matrix were uniformly illuminated with gamma rays and the coordinates reconstructed, each image pixel (with the same size as the crystal pixel) would have some events coming from gammas which interacted in the same pixel and some from gammas which interacted in adjacent ones. Assuming that the matrix is large enough, the total number of events contributing to an image pixel coming from surrounding pixels is also $N_{\text{wrong}}$. Therefore in any given image pixel the correct signal will be $N_{\text{right}}$ and the noise $N_{\text{wrong}}$.

B. Quality factor

$S/N$ is not sufficient to qualify a scintillator because efficiency is also important. The total number of interactions in a single detector multiplied by the $S/N$ ratio will give the total fraction of correctly reconstructed events. We therefore will also define a quality factor

$$
Q = \varepsilon \cdot (S/N).
$$

III. RESULTS

A. K-fluorescence emission and electron transport

In BGO scintillator, K-fluorescence X-rays and secondary electron range contribute to the misplacement of events in a reconstructed profile as can be seen in Figure 1 and Figure 2. In Figure 1 an extremely small pixel of 0.1 mm was chosen and the comparison is made with a 0.1 mm pixel YAP:Ce matrix. In these examples the thickness of the crystal was 0.2 GMFPs. We report the profiles for events with an energy selection: $E > 350$ keV for BGO and $E < 400$ keV for YAP:Ce. Figure 2 shows the same profiles as in Figure 1 but for a 0.2 mm pixel.

In both figures the fraction of misplaced events (defined as $F = N_{\text{Wrong}}/N_{\text{Tot}}$) and the value at the maximum are reported. Two things can be noticed. Firstly, although the total interaction probability in BGO and in YAP:Ce are the same (3.2% in coincidence) due to a thickness of 0.2 GMFP, the peak value of the profiles are significantly higher for YAP:Ce. This is because the photoelectric effect in BGO is 43% whereas the Compton probability in YAP:Ce is 96%. Having chosen high energy events for BGO with a thin crystal implies having chosen principally photoelectric events. Secondly the fraction of misplaced events is higher for BGO than for YAP:Ce due principally to the generally higher secondary electron kinetic energy and to K-fluorescence X-rays.

For 0.2 mm pixels the profile for YAP:Ce has significantly lower tails than for BGO.

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For 0.2 mm pixels the profile for YAP:Ce has significantly lower tails than for BGO.
B. Profiles for a 1 GMFP thick crystals.

In figure 3 and Figure 4 are reported the profiles of the reconstructed positions generated for $10^6$ 511 keV gammas incident on a slab of 1.04 cm thick BGO scintillator compared to a 2.18 cm thick YAP:Ce crystal (1 GMFP). All BGO events have an energy deposit greater than 350 keV (in both opposing detectors) whereas for YAP:Ce they are all less than 400 keV. Two different spatial pixelling are shown: 0.2 mm and 0.1 mm. The profile for YAP:Ce is narrower than for BGO. It can also be noted that as the spatial bin narrows, the peak efficiency of BGO decreases significantly whereas for YAP:Ce the peak efficiency is almost unaltered and for a 0.1 mm pixel the peak efficiency for YAP:Ce is higher than for BGO.

The fraction of misplaced events is $F_{0.5\text{mm}} = 52\%$ for BGO in the case of 0.5 mm binning, increasing to $F_{0.1\text{mm}} = 80\%$ for the 0.1 mm binning. In the case of YAP:Ce, the scatter fractions are respectively $F_{0.5\text{mm}} = 27\%$ and $F_{0.1\text{mm}} = 44\%$.

Figure 3: Profiles for the reconstructed position for a 1.04 cm thick BGO (bottom) scintillator and a 2.18 cm thick YAP:Ce scintillator (top). The spatial binning presented is 0.2 mm. All BGO events have energy deposit greater than 350 keV whereas for YAP:Ce they are below 400 keV. The fraction of misplaced events, $F$, is reported. The capabilities of YAP:Ce are superior to those of BGO.

Figure 4: Profiles for the reconstructed position for a 1.04 cm thick BGO (bottom) scintillator and a 2.18 cm thick YAP:Ce scintillator (top). The spatial binning presented is 0.1 mm. All BGO events have energy deposit greater than 350 keV whereas for YAP:Ce they are below 400 keV. The fraction of misplaced events, $F$, is reported. The capabilities of YAP:Ce are superior to those of BGO.

In Figure 5 a summary is reported showing the fraction of misplaced events $F = N_{\text{Wrong}}/N_{\text{Tot}}$ for the three scintillators considered as a function of pixel size in the two cases: without energy threshold (E>50keV) and with energy threshold (E>350keV for BGO and NaI(Tl); E<400keV for YAP:Ce). Furthermore results for NaI(Tl) are reported.

C. Uniformly illuminated pixel

To determine the signal to noise ratio for a scintillator detector to 511 keV gammas a single pixel was uniformly illuminate. The number of events reconstructed within the correct pixel and the number of events reconstructed in the
wrong pixel were determined. Again the thickness of the scintillators was 1 GMFP. Profiles of the ideally reconstructed coordinates were also determined.

In Figure 6 the profiles for 0.5 mm, 0.2 mm and 0.1 mm pixels are shown for BGO and YAP:Ce. The graphs show how the profiles for YAP:Ce are nearer in shape to the desired ‘box’ already for a pixel of 0.5 mm. The height of the profiles for BGO are higher but the S/N ratio is still favorable to YAP:Ce. More events are correctly placed within the pixel.

With a 0.2 mm pixel BGO and YAP:Ce have similar peak efficiencies but again YAP:Ce has a better S/N ratio due to fewer events being misplaced. Finally for 0.1 mm pixels BGO loses completely the desired ‘box’ shape and falls in height too. YAP:Ce on the other hand maintains a good profile showing good edges.

Figure 3. Ideally reconstructed profiles of events for a uniformly illuminated pixel within a 1 GMFP thick scintillator. 0.5 mm, 0.2 mm and 0.1 mm pixels are considered.

Finally in Figure 5 a graph comparing the quality factors for BGO and YAP:Ce is shown. Again we have also considered the two cases: without energy threshold and with.

Only for the 0.5 mm pixel and without an energy threshold does BGO outperform YAP:Ce.

Figure 5: Plot of the quality factor for BGO and YAP:Ce. BGO represents the highest Z material whereas YAP:Ce the lowest.

IV. CONCLUSIONS

Medium Z scintillators such as YAP:Ce show better spatial resolution capabilities than high Z scintillators, like BGO, due to the high single Compton scattering probability. In high Z materials, three contributions contribute to the deterioration of the reconstructed position; secondary electron range, K-shell fluorescence and, multiple Compton scattering within the scintillator. The fraction of scattered events in the case of a 0.1 mm binning are respectively $F_{0.1mm} = 80\%$ for BGO and $F_{0.1mm} = 44\%$ for YAP:Ce.

V. REFERENCES