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TITLE: Investigation of the CRT performance of a PET scanner based in liquid xe

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Report of referee 1

This paper describes the results from a Monte Carlo simulation of a PET system based on LXe cells instrumented with standard SiPMs (PETALO), and analyses the coincidence resolving time of the 511 keV gammas for this system under the assumption that the spacial resolution is 2 mm in both the depth of interaction axis and the perpendicular plane. In parallel, a similar system in which the LXe cells are replaced by monolithic LYSO crystals is simulated and directly compared with the PETALO system

It is not clear how the claimed spacial resolutions were estimated, as they do not agree with what is presented in the cited reference. Also, there is no discussion on how they may vary throughout the chamber. The results presented are heavily dependent on these resolutions, so they must be properly justified.

There are a few occasions in which the values quoted in the text do not agree with what is shown in the plots (as discussed below). The plot in figure 10 (of the velocity of the scintillation photons in LXe due to the variation of the refraction index with the wavelength in LXe) does not make sense considering what is described in the text and caption.

My opinion is that the discussions throughout the paper are biased towards concluding that the LXe cell has a better performance than the equivalent system using LYSO crystals, but a closer analysis of the plots presented,

under more realistic conditions, shows that that is not always the case (see more detailed discussions below).

I therefore recommend that the paper should not be published unless the errors indicated are corrected, the assumptions used in the simulation are more thoroughly discussed (spacial resolution, PDE of SiPMs to VUV light, TPB decay time), and the text is modified to have a fair comparison between the simulated LXe and LYSO setups.

General comments

- The subsections should be numbered, to make them easier to reference.
- The version of GEANT4 used for this work is never mentioned

Abstract

- The authors quote a CRT of 60-70 ps using VUV sensitive SiPMs, but this does not correspond to the conclusions obtained in the paper. Figure 13 shows a CRT of 70 ps for a PDE of 20% (which is currently not possible) and of 80 ps for a PDE of 15%. The same is true for SiPMs coated with TPB, for which the authors quote a value of 120 ps: the best value in the text is 130 ps, and that is considering a decay time of 1 ns for TPB, which the authors themselves indicate to have a typical range of 2.2 – 3 ns.

Section 2

- In the first subsection ("Physical properties..."), there is a reference to section 2 ("see section 2"). Section 2 is long and has several subsections, so this must be more specific.
- Also in this subsection, the authors mention that LXe has "an acceptable light attenuation length (36.4 cm)". It is not clear if this refers to the Rayleigh scattering interaction length, or to the absorption length by impurities in the xenon which varies greatly depending on the purity of the xenon. This has to be made clear, as the effects on the total light collection are completely different.
- In point 3 of the properties of xenon, a reference is needed when indicating a reduction of 2^{13} in the dark current of SiPMs at the temperature of liquid xenon

- At the top of page 4, a reference is needed at the end of the first sentence ("The relative contribution of SE and SR processes..."), even if it's the same used further below.
- after eq. 2.5, τ_r , the recombination time of the electrons, is quoted as being 15 ns for xenon. This is in contradiction with what is said in the previous page when discussing the two processes for producing scintillation light in xenon: here it is said that both processes (excitation and recombination) are of the order of the ps.
- once all the terms for eq. 2.1 have been obtained (up to eq. 2.6), it should be rewritten to provide a final equation for the points shown in figure 2.
- are the two time constants obtained from the fit (τ_1 and τ_2) the same as indicated previously for the singlet and doublet states?

Section 3

- The discussion on the concept of using LXe for a PET is written in such a way as to lead the reader to believe the Waseda group was pioneer in the area, which is not the case. The Coimbra group, for example, has work in this area since the early 90's.
- Figure 3 provides very little information to the reader, and can probably be removed. Maybe adding geometry information about the cell and the SiPMs simulated would make it more useful.
- Also in the caption of this figure, there is a sentence at the end saying "optionally also coated with TPB". This possibility is not discussed anywhere else in the paper, and must therefore be removed from here (or discussed in the text).
- On page 6, 2nd paragraph, "ASICs" is used without having been defined
- A spacial resolution of 2 mm in the xy plane seems hard to achieve using only a center-of-gravity algorithm in a 5 cm long chamber with the walls covered by high reflectivity PTFE. It must also vary along the z-axis and the xy plane, although that is not discussed here. Although there is a reference to a masters thesis, could the authors discuss in more detail how this resolution was estimated?

- Reference 11 indicates a resolution of 1.4 cm in both x and y directions (table 4) for a $3\times 3\times 5$ cm³ chamber. It is not clear from the caption of that table if this corresponds to the sigma of the gaussian fit or the rms, but comparing with the values shown in table 2 and figure 26 one can assume this is the sigma. The FWHM resolution is then 3.3 mm, not 2 mm. From figure 26 it is also clear that these resolutions were obtained for the center of the plane, and there is no mention of how they degrade for positions closer to the walls. Moreover, there is no discussion of how the xy resolution varies along the z axis.
- The same is true for the DOI: table 4 in ref 11 shows a resolution of 1.4 mm for a $3\times 3\times 5$ cm³ (no mention of the position inside the chamber that was used to estimate this value), which also corresponds to 3.3 mm. It is also clear from figure 25 that this resolution must vary along the z axis, but this is not discussed.
- It should be noted that on the last paragraph of page 6, the authors mention that "Further improvements [...] eventually result in a PDE of 20%" for VUV-SiPMs, but use this as the benchmark value for most discussions throughout the paper.
- Also noteworthy, at the top of page 7 the authors indicate that the decay constant of TPB has been measured to be between 2.2 and 3 ns, but later quote CRT values considering a decay time of 1 ns without proper justification.

Section 4

- The GEANT4 version used for this study is never mentioned
- The size and pitch of the SiPMs is not indicated
- When discussing the Rayleigh interaction, one should use "interaction length", and not "attenuation length". The light is merely scattered, not absorbed.
- At the end of page 7, when discussing the effect of coating the SiPM windows with TPB, I don't understand why the xenon refractive index is considered again. Light emitted by the TPB coating will go directly into the SiPM window, so what is relevant here is the TPB refractive index.

- In figure 5, the black background should be removed. Also, in the caption of the figure, the direction of the gammas is irrelevant to the user.
- It would be much more useful for the discussion to show a schematic representation of the distances discussed on page 8 to obtain the Δt equation (4.2) than a figure from the simulation that provides no relevant information.
- On page 9, 2nd paragraph in subsection "Intrinsic CRT...", I don't understand what is the x in the equation shown inline with the text $(n \cdot x \cdot d_p / c)$ – and it is not in the caption of figure 7, where this equation is shown again
- In the beginning of the last paragraph on page 9, I think it is not Δd_p , but only d_p
- I have some doubts about the usefulness of figure 7, as this is just a consequence of the decay time of the scintillation light.
- The size of the SiPMs is only mentioned in the caption of figure 7, never in the main text.
- I don't understand the discussion at the top of page 10 about the DOI resolution for a 20 mm thick LYSO crystal being given by a "digital resolution". Could the authors elaborate on this and maybe provide a schematic figure?
- At the end of the "Intrinsic CRT" subsection (page 10), the authors compare the intrinsic CRTs that were obtained for LXe and LYSO, using a PDE of 20% for the VUV SiPMs in the case of xenon to conclude that the intrinsic CRT is better (30 ps compared with 45 ps for LYSO). But as discussed by the authors before, VUV SiPMs with 20% PDE do not exist yet. The fair comparison is using a PDE of 15%.
- Figure 10 does not make sense. The refraction index of liquid xenon for the mean scintillation wavelength is 1.7 (which corresponds to a velocity of 0.176 mm/ps), while the extremes of the distribution correspond to values of n of 1.58 and 2.1 approximately (resulting in velocities of 0.19 mm/ps and 0.143 mm/ps respectively). The velocity distribution shown is both wider than it should, and the mean is completely off.

- For the value of the fraction of photons transmitted through the SiPM window, is this the average value obtained from the full simulation (and thus having a realistic angular distribution, wavelength spectrum and corresponding refraction index) or is it estimated using an n of 1.7 only? This should be made clear.
- Again, when comparing the CRTs of LXe and LYSO at the end of the subsection where the effects of refraction index are included, the authors use a PDE of 20% in the case of LXe. If using the CRT value at 15%, the CRT in LYSO is already smaller than that of xenon.
- In the comparison between the CRT values of LXe and LYSO after introducing the effect of the jitter in the SiPMs and front-end electronics, the values quoted do not correspond to the values in figure 12: it is said that for LYSO with a PDE of 50% the CRT is 125 ps, while it is in fact 115 ps in figure 12; also, it is said that the CRT in LXe is " ~ 100 ps" for a PDE of 20%, while it is in fact 110 ps. Using a PDE of 15% for LXe, the CRT is 115 ps, so the same as LYSO for a PDE of 50%.
- When considering the average arrival time of the first 10 photons, the fair comparison is 85 ps for LYSO (with a PDE of 50%) and 80 ps for LXe (for a PDE of 15%)
- In the caption of figure 15 it should be clearly stated that the effect of the jitter in the SiPMs and the electronics is not included.
- A plot should be added showing the CRT for TPB coated SiPMs and including the effect of the jitter in the SiPMs and front-end electronics (this could be done for a PDE of 50% only).
- The best CRT using TPB is obviously considering a decay time of 1 ns, but the authors themselves quote a range of 2.2 – 3 ns for observed decay times with TPB. If one considers the more realistic 2.2 ns decay time, the CRT in LXe is then 155 ps (considering the average of the first 10 photons), which should be compared with the 85 ps obtained for LYSO in the previous section (or even 115 ps considering only the first photon).

Section 5

- I don't understand the discussion about the intrinsic resolution of 12 ps of which the DOI uncertainty contributes with 10 ps: in the respective section it is said that the DOI contributes with 11.2 ps, and the value 12 is never mentioned. Does this come from the width of the curves in figure 8? If so, it must be mentioned in that section.
- The authors conclude that a LXe system could have a CRT smaller than 100 ps, but the same is true when using the LYSO crystal in the same conditions, as also shown in this work.
- When discussing the results for TPB coated SiPMs, the authors again use the range 1 – 2.2 ns for the decay time, not the 2.2 – 3 ns they cite as having been measured. The result obtained with the monolithic LYSO crystal and conventional SiPMs in this work is better than the CRT for a 2.2 ns TPB decay time by almost a factor of 2 (85 ps VS 155 ps)

Report of referee 2

I think the paper has a high scientific quality and deserves publication, but I have some minor comments.

I do not understand Fig. 10. You say it comes from convolving Fig. 1 and 6. From Fig. 1 wavelengths are between 160 and 220 nm; looking at Fig. 6. these correspond to refraction indices between 2.1 and 1.5, so the speeds should be between $0.3/2.1$ and $0.3/1.5$ mm/ps and in Fig. 10 they are quite lower.

Page 10: $20/\sqrt{12}$ is not 13.3 but 5.8. This is indeed the number you have used to get 34 ps.

Page 12: I do not understand why the CRT in LYSO is 125 ps and in LXe 100 ps. I guess you have added to the 50, 80 and 30 ps plus a DCR; but with a DCR of 85 that you quote in page 2, you get 130 ps, not 125 ps.

I am missing a plot of the final CRT with all factors included as a function of the number of photoelectrons. As this is the final numbers you get, I would be very illustrative.

Editor's comments

I would like to ask the authors to carefully check the paper for consistency (e.g. the values of resolution in the abstract do not coincide with those in Conclusions; also, there is apparently some divergence between the text and some plots as noticed by the reviewers). I have also a few particular comments.

- P.3, 3rd line: reasonable — correct to *reasonably*
- P.6, paragraph on spatial resolution of LXSC2. I think details of the simulated cell should be given here (e.g. dimensions, SiPM pixel size, PDE) to help the reader. It is also important to mention that the presented results come from Monte Carlo simulations. Please, specify whether 2 mm resolution (in x,y and DOI) is for a specific point inside the cell, average or the whole volume.
- Fig 4 is a direct reproduction from another paper and may rise copyright questions. A permission has to be asked from Elsevier and the authors (then it should be mentioned in the figure caption ‘published with permission from Elsevier’). Alternatively, you might consider modifying the figure.
- Beginning of section 4 where the simulated setup is described. Please, specify SiPM pixel size. In general, I think, it would be useful to make a table with the setup specification as well as the values of the parameters used in the simulations.
- P.9 last paragraph — p.10 first paragraph. Comparison with LYSO is very much confusing in my opinion. It looks like you are comparing two different configurations — SiPMs on both sides of the scintillation cell for LXe and LYSO monocrystal with sensors on one side only. I do not quite understand what conclusion can be derived from that (at least not in favour of LXe, if any). The third case ‘conventional segmented LYSO crystal’ looks even more confusing. What is ‘conventional segmented ... crystal’? From calculations that follow it looks like it is not segmented at all (by the way, sensors on one side or on both? not pixelized I suppose?). If this is the case, it seems obvious that its time

resolution will be worse because there is no possibility of position correction. Besides, I continue to doubt in correctness of invoking digital resolution to prove that. Do you really need this example?