Metascintillator pulse shape analysis for optimizing energy and timing measurements

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Abstract

The working principle of metascintillators is based on sharing the energy of an impinging gamma ray between their composing materials. Such can be a dense crystal such as LYSO or BGO to maximize the gamma stopping potential and a fast organic or inorganic compound such as BC-422, EJ232 or BaF2 for its light production kinetics. In this work we look into the details of metascintillator pulses as modelled through a double bi-exponential model. We analyze the extent of energy sharing, as understood through analysis, simulation and experiment in a coincidence timing resolution (CTR) measurement setup, using 3x3x15 mm3 metascintillators, against a reference detector. Features of individual pulses allow choosing the photoelectric interactions and provide insight on the energy sharing extent of each gamma interaction. We evaluate the quality of energy sharing surrogates for different metascintillator designs. Different populations of photoelectric interactions depending on the extent of energy sharing are defined, that have different contribution of fast photons in the first picoseconds and hence different timing. We benchmark this selection through using these features to apply a timewalk correction on an event-to-event basis. A significant improvement is demonstrated in all cases, while for a 3:1 volume ratio BGO:EJ232 metascintillator this improvement rises up to ˜25% for the whole photopeak (204.7 ps), while the 10% events with higher production in the fast emitter show a ˜50% improvement to 54.7 ps. This shows that while metascintillators with comparable light yield components still provide the best alternative, it is possible through simple pulse analysis to measure and isolate the photoelectric interactions in every metascintillator with two components

Metascintillator pulse shape analysis for optimizing energy and timing measurements

Georgios Konstantinou, Riccardo Latella, Laura Moliner, Lei Zhang, Jose Maria Benlloch, Antonio J. Gonzalez, *Member, IEEE*, Paul Lecoq, *Fellow, IEEE*

***Abstract*— The working principle of metascintillators is based on sharing the energy of an impinging gamma ray between their composing materials. Such can be a dense crystal such as LYSO or BGO to maximize the gamma stopping potential and a fast organic or inorganic compound such as BC-422, EJ232 or BaF_2 for its light production kinetics. In this work we look into the details of metascintillator pulses as modelled through a double bi-exponential model. We analyze the extent of energy sharing, as understood through analysis, simulation and experiment in a coincidence timing resolution (CTR) measurement setup, using 3x3x15 mm^3 metascintillators, against a reference detector. Features of individual pulses allow choosing the photoelectric interactions and provide insight on the energy sharing extent of each gamma interaction. We evaluate the quality of energy sharing surrogates for different metascintillator designs. Different populations of photoelectric interactions depending on the extent of energy sharing are defined, that have different contribution of fast photons in the first picoseconds and hence different timing. We benchmark this selection through using these features to apply a timewalk correction on an event-to-event basis. A significant improvement is demonstrated in all cases, while for a 3:1 volume ratio BGO:EJ232 metascintillator this improvement rises up to ~25% for the whole photopeak (204.7 ps), while the 10% events with higher production in the fast emitter show a ~50% improvement to 54.7 ps. This shows that while metascintillators with comparable light yield components still provide the best alternative, it is possible through simple pulse analysis to measure and isolate the photoelectric interactions in every metascintillator with two components.**

***Index Terms*— CTR, DTR, PET, scintillators, TOF**

I. Introduction

IMPROVING the coincidence timing resolution (CTR) in PET systems is actively nowadays being pursued, since the addition of time-of-flight (TOF) information increases the system effective sensitivity. A growing trend concerns multiple timing kernel events due to multiple mechanisms of photon production [1]. This is the case for Cherenkov-light based timing approaches, but also for metascintillator designs [2]. Metascintillators refer to the combination of a high-Z scintillating crystal (HZ), such as LYSO or BGO which provides the stopping power, with faster emitting (FE) scintillators such as organic scintillators or BaF_2, that are sampled spatially at a submillimeter scale, at least in one dimension. Due to the close proximity between the two materials, these share the low energy optical photon production through a stochastic energy sharing function. This function reflects the trajectory and range of the recoil electron produced through the interaction of the 511 keV gamma quantum with the scintillating material. The resulting metascintillator reaches improved timing, caused by the multitude of photons produced with the kinetics of the fast material, without sacrificing the overall stopping power of the detector, which sprouts from the existence of a high-Z material.

Nevertheless, the combined photon production and the stochastic character of energy sharing add an extra challenge in defining not only the detector timing resolution (DTR), but also the application of detectors with variable DTR per event, in the PET image reconstruction process. This process is one that can reflect to all multi-kernel timing systems and will be the focus of this work, in the case of metascintillators.

II. Materials and Methods

A. Metapixels

In order to evaluate the potential of such systems, we constructed a number of metapixels, corresponding to metascintillators with dimensions such that coupling to SiPM is similar to that of pixelated detectors. These are composed by thin (≤0.3 mm) slabs placed on top of each other. In previous works [2][3] we have demonstrated how the volume ratio of the composing scintillators affects energy sharing. The general analysis of energy sharing does not change regardless of the scintillator topology chosen, hence we focus this work on metapixels of external dimensions of 3x3x15 mm^3, wrapped in Teflon. We built and tested several metapixels, mostly based on BGO as the high-Z material, using EJ232, EJ232Q-0.5% Benzophenone and BaF_2 as FE, with volume ratios from 3:1 to 1:1 HZ:FE. On top of that, we built a 2:5 LYSO:BC422 metapixel to evaluate LYSO as the HZ material, which also has significant production of photons in the first nanoseconds.

B. CTR test bench

These metapixels were tested against a LYSO:Ce:Ca reference detector (SIPAT, 3x3x5 mm^3) on FBK 3x3 mm^2 NUV SiPM with resulting 78 ps DTR, in a test setup with two readout channels, one using a Balun transformer circuitry [4] and three stages of amplification for a fast timing signal, and a second one for energy measurement (see Fig. 1). The read-out was based on a 8GHz Rhode-Schwarz oscilloscope. While the electronics are designed for high timing precision, suitable for TOF

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purposes, the main purpose of this setup is to understand in detail the characteristics of metascintillator pulse response and how this can be used in system scale development, rather than achieve a CTR similar or better compared to the state of the art.

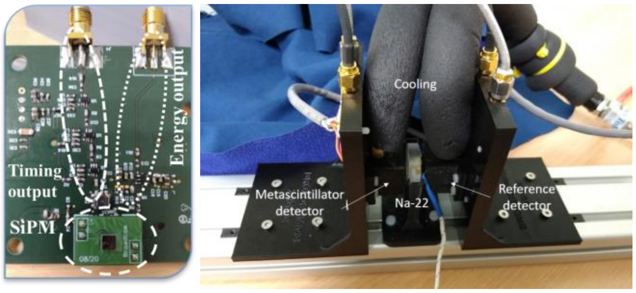

Fig. 1. (Left) The developed circuit, comprising a broadband, Balun and RF electronics based timing channel and a conventional energy channel; and (right) the CTR measurement setup with air cooling channels.

C. *Energy sharing and the quad-exponential model*

HZ and FE scintillators have different time coefficients in their photon production, while they also tend to have different light yields. Each produces photons independently according to the bi-exponential model [3]. The metascintillator photon production corresponds to the addition of the production of the two materials (eq. 1).

$$f_{metascint}(t) = \frac{E_{fe} \times LY_{fe}}{\tau_{fed} - \tau_{fer}}\left(e^{-\frac{t}{\tau_{fed}}} - e^{-\frac{t}{\tau_{fer}}}\right) + \frac{E_{hz} \times LY_{hz}}{\tau_{hzd} - \tau_{hzr}}\left(e^{-\frac{t}{\tau_{hzd}}} - e^{-\frac{t}{\tau_{hzr}}}\right) \quad (1)$$

where E stands for energy, LY for light yield, τ for time coefficients, fe subscripts correspond to the kinetics of the FE scintillator, hz to those of the HZ one, r to rise and d to decay coefficients.

Looking at this quad-exponential model, it is clear that the standard approach of using an energy filter to isolate the photopeak is not applicable. In particular, the measured effective light yield, as retrieved from the SiPM output corresponds to eq. 2:

$$LY_{effective} = \frac{E_{hz} \times LY_{hz} + E_{fe} \times LY_{fe}}{E_{hz} + E_{fe}} = \frac{LY_{hz} + \frac{E_{fe}}{E_{hz}} \times LY_{fe}}{1 + \frac{E_{fe}}{E_{hz}}} \quad (2)$$

The interaction energy corresponds to $E_{hz} + E_{fe}$, while the ratio $\frac{E_{fe}}{E_{hz}}$ corresponds to the energy sharing. Through this we see that shared photoelectric interactions can have an effective light yield in the same region as the Compton scattering of the HZ scintillator. This is the case for both LYSO: EJ232 and BGO:EJ232Q configurations. BaF_2 has a slightly higher total light yield compared to BGO and EJ232 has effectively the same light yield, making data selection more trivial.

This means that especially when the two materials do not have a comparable light yield, we need to measure the total energy while in the same time estimate the amount of energy released in the HZ and the FE scintillators, in order to isolate photoelectric from Compton interactions. For this reason, we require two independent energy surrogate measurements. Such can be different features of the pulse, such as the maximum value or the rising slope, or integration with different windows.

D. *Light yield time series*

Some features have already been researched [5] and provided sufficient information concerning energy sharing. However, we chose to focus on the double integration approach, as it can be easily applicable in existing systems, that already commonly use integration in order to evaluate pulse energy. In figure 2, we compare the light production of composing scintillators over time, in the case of BGO and.EJ232Q-0.5% (left) or EJ232 (right). We see that for the extreme cases of events taking place exclusively in the one or the other material, the ratio of emitted photons follows an easily traceable distribution. EJ232Q light is released in the first few nanoseconds, while the light of BGO lasts up to almost 1 us. The two materials have released substantially the same amount of photons around 90 ns after scintillation onset. This means that at this point the integral should be distributed in a histogram largely similar to that of standard scintillators, albeit with the measurement uncertainty caused by the relatively small light yield up to this point, equal to that of the FE.

Every integral that is smaller than 90 ns, will lead to a histogram where the strongest events correspond to those with highest energy sharing. We chose an integration window of 50 ns to compromise between a strong ratio, substantial number of photons and the limited bandwidth of the readout circuit.

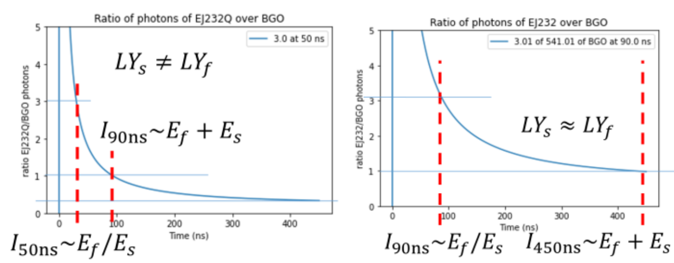

Fig. 2. (left) ratio of total produced photons between EJ232Q and BGO as it develops over time. When this ratio crosses 1, energy sharing is not visible in the integral histogram, while when this ratio is more than 1, strongly shared events are favored according to the ratio value; and (right) when the light yields are substantially the same, the ratio converges to 1 with time.

E. *Application of timewalk correction*

To research how this analysis can be applicable to identify these events, we proceeded in a series of acquisitions of different metapixels against a reference of 3x3x5 mm^3 LYSO:Ce:Ca (SIPAT, China) with 110 ps CTR. The time resolution of the reference is unfolded from the metapixel timing through its pythagorian relation to reach the intrinsic CTR, the CTR value in the case of a coincidence experiment of two same metapixels. Post-acquisition analysis took place in Python. In previous works [2][3], a comprehensive study of the nature of energy sharing has been provided, based on Monte

Carlo simulations. Moreover, the performed pulse analysis demonstrated that shared events have an increasingly faster response related to the number of produced fast photons. This knowledge serves as the theoretical basis for an exponential time-walk correction approach, which can be applied through the energy sharing or any surrogate feature (measured pulse energy or maximum value) [2].

The possible improvement that timewalk correction can provide corresponds to the quality of energy sharing discrimination provided through this analysis. A choice of a percentage of faster events is possible as these events correspond to only strongly shared ones.

III. Results

A. *Energy resolution of the gated approach.*

If we analyse equation 2, integrate it for the proposed integration windows τ_{int} and take into account certain premises ($\tau_{int}>>\tau_{fed}$, $\tau_{int}>>\tau_{fer}$, $\tau_{int}>>\tau_{hzr}$, $\tau_{hzd}>>\tau_{hzr}$), we obtain equations 3 and 4:

$$\begin{aligned} I(E_{fe},E_{hz},\tau_{int}) &= \int_0^{\tau_{int}} f_{metascint}(t)dt \\ &= \int_0^{\tau_{int}} \left\{ \frac{E_{fe}\times LY_{fe}}{\tau_{fed}-\tau_{fer}}\left(e^{-\frac{t}{\tau_{fed}}}-e^{-\frac{t}{\tau_{fer}}}\right) \right. \\ &\left. + \frac{E_{hz}\times LY_{hz}}{\tau_{hzd}-\tau_{hzr}}\left(e^{-\frac{t}{\tau_{hzd}}}-e^{-\frac{t}{\tau_{hzr}}}\right)\right\} dt \\ = \frac{E_{fe}\times LY_{ef}}{\tau_{fed}-\tau_{fer}} & \left(-\tau_{fed}e^{-\frac{\tau_{int}}{\tau_{fed}}}+\tau_{fer}e^{-\frac{\tau_{int}}{\tau_{fer}}}+\tau_{fed}-\tau_{fer}\right) \\ &+ \frac{E_{hz}\times LY_{hz}}{\tau_{hzd}-\tau_{hzr}}\left(-\tau_{hzd}e^{-\frac{\tau_{int}}{\tau_{hzd}}}+\tau_{hzr}e^{-\frac{\tau_{int}}{\tau_{hzr}}} \right. \\ &\left. + \tau_{hzd}-\tau_{hzr}\right) \end{aligned} \quad (3)$$

$$I(E_{fe},E_{hz},\tau_{int}) = E_{fe}\times LY_{fe} + E_{hz}\times LY_{hz}\left(1-e^{-\frac{\tau_{int}}{\tau_{hzd}}}\right) \quad (4)$$

This demonstrates that all necessary information to evaluate the energy of interaction, in order to push the quality of energy resolution of metascintillators to that of normal scintillators are present; however, two integrations are needed per pulse. This is furthermore a simple approach that can be easily implemented in hardware or firmware at the front-end of the metascintillator detector.

B. *Photoelectric interactions and energy sharing for different light yields*

The fast output of the circuit carries the information of the max value of the pulse, which is bigger for shared events than LYSO events of the same energy. Furthermore, the effective light yield of shared events is smaller than that of LYSO events. The combination of these features allows discrimination of the energy and energy sharing of individual events (Fig. 3).

In this plot, logarithmic iso-sharing lines and slightly exponential iso-energy lines provide the required information. The limit of this analysis is the resolution of the respective measurements

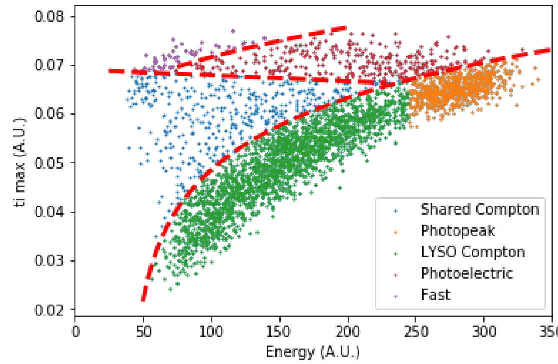

Fig. 3. XY scatter plot of events according to their total energy and max value of the fast response channel and demonstration of the different populations depending on their energy released in the FE (0-photopeak, less than 130 keV-shared, more than 130 keV -fast)

C. *Photoelectric interactions and energy sharing for the same light yield*

For the 3:1 BGO:EJ232 configuration we used the approach of double integration with different integration windows. As the light yield of the corresponding metascintillators equalizes at the end of the pulse. Using this information, we are able to isolate the photoelectric interactions in the traditional way (integration gate at 450 ns), while a second integration at 90 ns provides a strong surrogate of the energy sharing. The scatter plot presented in figure 4 shows significant agreement with the energy sharing as simulated previously [3], which is overlaid on the plot.

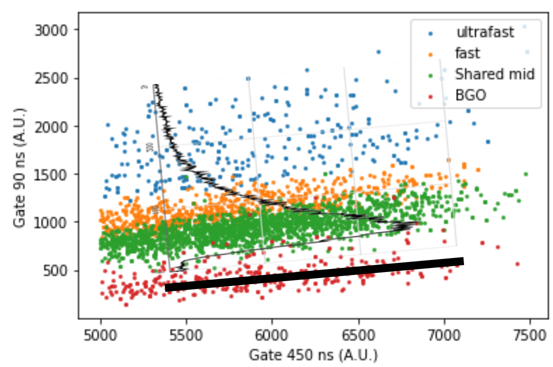

Fig. 4. XY scatter plot of photopeak events of a 3:1 BGO:EJ232 metapixel, demonstrating good agreement with the overlaid simulated energy sharing distribution, allowing the definition of event subsets.

D. *Metascintillator time-walk application*

The example presented here corresponds to a 3:1 BGO:EJ232 metapixel. Similar approaches have been undertaken for all tested metapixels. The discriminating feature used was the integral at 90 ns. A linear fit was tried to shift the mean value of all sub-groups of events in the same value. The CTR is significantly reduced from 280.1 ps to 204.7 ps. Moreover, the square root error residue is significantly reduced after the correction.

The timewalk correction is more significant for the subgroup of ultrafast events, as they correspond to a small population of highly variable energy sharing. Here, the intrinsic CTR of such events is reduced almost by half from 106.2 ps to 54.7 ps. Better timewalk correction can present better results, as demonstrated by the fact that the bump at the right side is not totally eliminated.

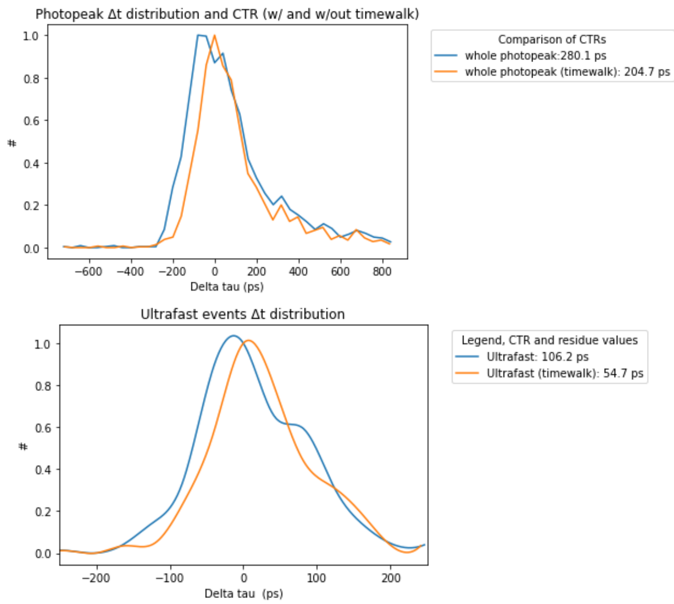

Fig. 5. Δt distributions from the 3:1 3x3x15 mm^3 BGO:EJ232 metapixel: (top) the whole photopeak is fitted with a hybrid Gaussian-Laplacian fit before and after timewalk correction; and (bottom) A 9.5% of chosen shared events, corresponding to the blue population of figure 4, fitted with a hybrid Gaussian-Laplacian function before and after timewalk correction.

The results from different metapixels are collectively presented in table 1. Choice of a highly shared subset is easier when light yields are closer to each other, which leads to generally better energy sharing characterization and consecutive improvement on timing by the timewalk correction algorithm.

TABLE I

CTR RESULTS WITH THE APPLICATION OF TIMEWALK CORRECTION

Metascintillator type	CTR W/ REFERENCE	INTRINSIC CTR	SUBSET %	SUBSET INT. CTR
BGO/EJ232	164.3 ps	204.7 ps	9.5%	54.7 ps
BGO/BaF2	190.5 ps	241.2 ps	13%	108.5 ps
BGO/EJ232Q	176.1 ps	223.4 ps	17.4%	141.4 ps
LYSO/EJ232	133.7 ps	153.8 ps	6%	93.5 ps

IV. DISCUSSION-FUTURE PLANS

Through this analysis we demonstrate that defining both the interaction energy to isolate the photoelectric events and energy sharing to organize them in subsets is possible both for metascintillators with the same and different light yield in their composing materials. This study will have to be slightly adapted for new materials and more complex metascintillators, while it can support different readouts on a system level development. It is clear that if light yields are the same or close to each other the analysis renders better results, as the features to be used for energy sharing discrimination are more robust.

The precision with which energy sharing can be predicted is demonstrated by the application of a first order timewalk correction algorithm, which significantly improves the overall CTR of the measured topologies. Higher order algorithms will be attempted and the same benchmarking process will be repeated.

Those preliminary results demonstrate that the addition of fast emitters can significantly improve the timing of both LYSO and BGO based detectors after using an easily implementable timewalk correction, with a subset of the shared events reaching up to 50% improvement. In particular for the 3:1 BGO:EJ232 metapixel, we achieve an overall CTR better than the state of the art with similar sensitivity, but with a significantly lower cost of scintillators, given that BGO is 3 times cheaper than LYSO and EJ232 up to 5 times. In the same time, for a subset of these events we achieve a CTR half from our 3x3x5 mm^3 LYSO reference on the same electronics. These fast events can successfully guide the reconstruction of a PET image with improved ToF capabilities further adding to the effective sensitivity of the metascintillator based system.

Measurements with different composite metascintillators are taking place to assess the effect of parameters such as the scintillator mass ratio, volume, length and fast emitter material, on the effective CTR. The energy resolution of the measurement setup plays a significant role in the precision of event selection and a new optimized setup is being commissioned. At the moment, the features used are the ones demonstrated in previous works. Other features, such as the slope, are to be further analyzed. Machine learning will be applied on the retrieved datasets to provide better resolution for the energy sharing estimation. As the photon production mechanisms are being further understood, the next significant step in the metascintillator quest for optimized timing, is to address the limitations of light propagation.

These encouraging results with pixel styled detectors lead the way for further development in topologies that can be applicable on the system level, either in pixelated or monolithic/semimonolithic approaches. The interplay between the presence of faster subsets of events also has to be evaluated through direct metascintillator to metascintillator CTR studies.

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