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Optical and scintillation properties of Lead Tungstate crystals: a statistical approach

I. Dafinei[1]

CMS Collaboration

Abstract

The Compact Muon Solenoid (CMS) is one of the five experiments foreseen at the Large Hadron Collider at CERN. The Electromagnetic Calorimeter (ECAL) of CMS will be the largest crystal calorimeter ever constructed. Over 34000 lead tungstate (PbWO4) crystals representing more than half of the barrel part of the ECAL were fully analyzed till present for their optical and scintillation properties as a part of the ECAL modules construction activity. This huge quantity of information may also be used in order to emphasize general properties of the material and find possible correlations between optical and scintillation parameters measured on large crystals produced at industrial scale. Such correlations proved to be useful tools for the crosscheck between LY and optical transmission measurements, the improvement of the ECAL crystals inter-calibration precision and for tuning the quality of crystals produced at industrial scale.

Some comments, function of the type of paper, may be inserted here:

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[1] Università "La Sapienza", Dipartimento di Fisica and INFN Sezione di Roma, P-le Aldo Moro 2, 00185-Roma, ITALY

1 Introduction

$PbWO_4$ (PWO) crystals used for the construction of the electromagnetic calorimeter (ECAL) of the CMS experiment at CERN [1] undergo several tests following the qualification procedure defined by the CMS Collaboration [2]. Crystal characteristics are measured to ensure the performance of ECAL detector, tune the quality of crystals produced at industrial scale and will serve the ECAL exploitation, mainly in commissioning and starting-up phases. These data are also suitable for statistical analysis aimed at giving hints on scintillation characteristics of large PWO crystals, otherwise impossible to be put in evidence (direct measurements are out of discussion given the dimensions and number of crystals). Recent analysis [3] evidenced a strong correlation between crystal light yield (LY) and longitudinal transmission (T) in the range 350-370 nm which opens new opportunities to improve the intercalibration of crystals, a key point for a successful start-up of the CMS experiment. Understanding the intimate mechanism of this correlation is the main purpose of the present work.

2 Optical parameters statistics

PWO crystals under discussion were produced in Russia. The following analysis refers to all delivery kfdkjfhkjfhk ajkdfhakfhakfhfk jkddkjkjndkjfn batches containing a statistically significant number of crystals (N>20), i.e. 11564 of the 11696 processed with REDACLE database [4] at ECAL-CMS Regional Center of INFN located at ENEA-Casaccia Rome, Italy. Fig. 1 gives the range of values of T and LY for these crystals.

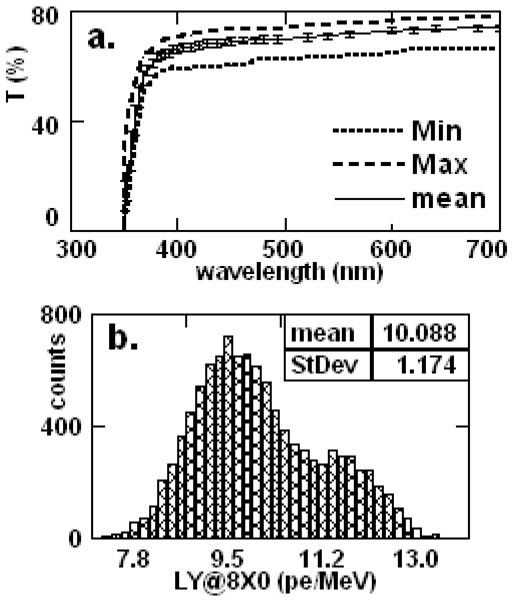

Figure 1: Optical transmission (a) and light yield (b) of 10598 PWO crystals studied in this work.

The correlation factor between T and LY for a set of N crystals, defined as:

$$C_{T-LY}(\lambda) = \frac{\sum_{j}^{N}\left(T_j(\lambda) - \overline{T}(\lambda)\right)\cdot\left(LY_j - \overline{LY}\right)}{N\cdot\sigma_T\cdot\sigma_{LY}} \qquad (1)$$

should be influenced by the two processes involved in the light yield, i.e. the scintillation light production and the light transport. A maximum correlation is expected around the PWO scintillation peak at 420 nm. However, the strongest correlation was noticed in a sharp wavelength region around 360 nm for all crystals batches analyzed. Fig. 2 gives the spectral correlation for all crystals and for two separate batches randomly chosen from the set of 23 studied in this work.

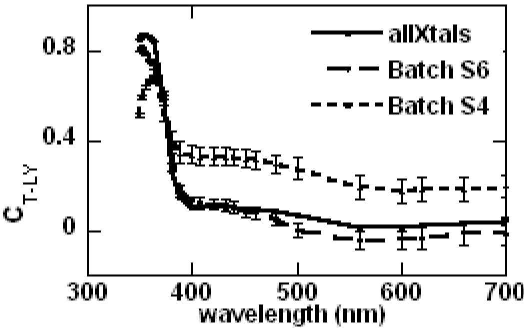

Figure 2: Correlation between light yield and longitudinally measured transmission for different batches of PWO

Taken into consideration the transparency of a crystal in a given wavelength range:

$$\tau(\%) = \frac{1}{\lambda_2 - \lambda_1} \cdot \int_{\lambda 1}^{\lambda 2} \mathrm{T}(\lambda) \cdot \mathrm{d}\lambda \qquad (2)$$

the contribution of light transport to the T-LY correlation was further investigated through the mean transparency of a batch of crystals <τ>, in connection with the average LY of crystals in that batch, <LY>. As figure 3 shows, for the 23 crystal batches studied in this work there is a very strong correlation between <LY> and $<\tau>_{350\text{-}375\ \mathrm{nm}}$ in spite of the poor relative weight of the scintillation light emitted in 350-375nm spectral region (7% of the total scintillation light). On the other hand there is no correlation between <LY> and $<\tau>_{400\text{-}440\ \mathrm{nm}}$ though 31% of the scintillation light is emitted inside the 400-440 nm spectral range. This anomalous connection between <LY> and <τ> plus relative weight of scintillation emitted in a given wavelength range is a clear proof that light transport in PWO crystals is not the driving factor of the T-LY correlation under discussion.

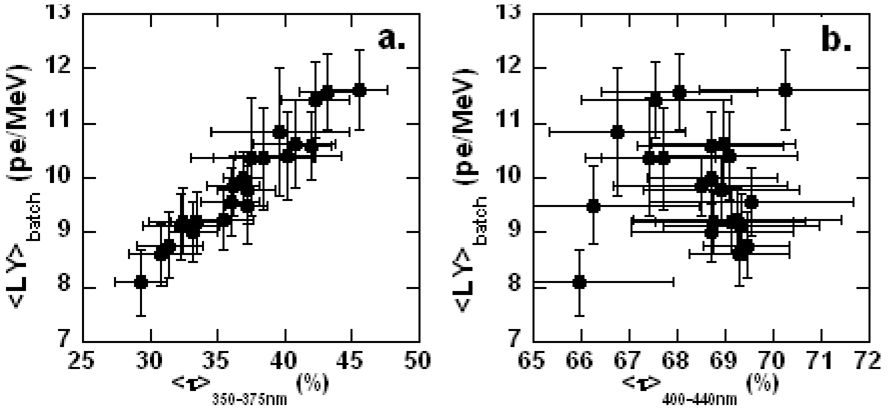

Figure 3: Correlation between mean values of *LY* and transparency in two different wavelength regions for the 23 crystal batches studied in this work: a) 350 - 375 nm and b) 400 – 440 nm regions, where 7% and respectively 31% of the PWO scintillation light is emitted.

Before we start searching for the origin of T-LY correlation in PWO crystals, it is to be mentioned that this material is a "tunable" scintillator [5], i.e. its scintillation properties can be modified through crystal doping and/or modifications of the crystal growth technology. The drawback of this peculiarity consists in a relatively limited possibility to control the scintillation and optical transmission parameters along crystal ingots and from crystal to crystal inside batches of crystals grown in the same conditions. One should expect therefore to have small variations of these characteristics along as-grown crystal ingots and a spread of scintillator parameters from crystal to crystal inside large batches of industrial production. For what concerns transmission characteristics, there are several reasons to have such variations, from simple differences in the polishing quality or non-homogeneities of the refractive index to the presence of color centers or extended crystal defects. Concerning the scintillation characteristics, it is well established that ideally there are two components in PWO luminescence spectrum namely a "blue emission" centered around 420 nm (ascribed to $(WO_4)^{2-}$ regular lattice centers) and a "green emission" centered in the 480-520 nm spectral region (ascribed to WO_3 defect center) [6]. Real, possibly doped crystals may have deviations from the ideal situation concerning the relative concentration and effectiveness of these two emission centers. As a consequence, the overall emission spectrum of PWO crystals having different composition (doping) and grown with different technologies, may vary in green/blue intensity ratio and overall spectrum position and intensity. However one has to bear in mind that PWO crystals under discussion are specially produced for ECAL use, result of a dedicated R&D activity aimed among other goals at removing the green slow component and enhance the regular centers contribution to the scintillation spectrum. It is therefore expected that only small variation of overall spectrum intensity should be present in the crystals under discussion.

3 Semi-empirical model

The light yield of a PWO crystal will be intended in the following as value of the parameter LY@8X0 defined by ECAL-CMS collaboration [1, 2]. In the frame of a simple model it may be calculated using the formula:

$$LY = c\cdot\int S(\lambda)\cdot \mathrm{T}^{\mathrm{n}}(\lambda)\cdot\varepsilon_{\mathrm{PM}}(\lambda)\,\mathrm{d}\lambda \tag{3}$$

where $S(\lambda)$ is the scintillation spectrum, $T(\lambda)$ the transmission, n the effective path of the light inside the crystal expressed in crystal length units, $\varepsilon_{PM(\lambda)}$ the quantum efficiency of the photo-detector and c is a calibration constant. The intensity of the scintillation spectrum depends on the concentration of effective luminescent centers:

$$S(\lambda) = (\mathrm{n}_0 - q\cdot n_t)\cdot f(\lambda) \tag{4}$$

where n_0 is the concentration of luminescent centers, n_t concentration of centers acting as effective traps for secondary carriers generated by gamma excitation in the scintillation process [7], q trapping quantum efficiency and $f(\lambda)$ is a distribution function whose nature and properties are not the subject of this work and considered to be the same for all PWO crystals under study. Trapped carriers, even if are further thermally released, will recombine non-radiatively rather than transfer the corresponding excitation to a scintillation center, thus being lost for the scintillation process. Some of the trapping centers may put their fingerprint in the region of the absorption band edge of the transmission spectrum of PWO crystals [6]. For wavelengths values above the fundamental absorption edge, the absorption coefficient α depends practically only on the concentration of impurities and may be written as:

$$\alpha(\lambda_0) = \alpha_0 = const\cdot(n_t - n_b) \tag{5}$$

where nb is the concentration of other absorption centers active at the same wavelength λ_0.

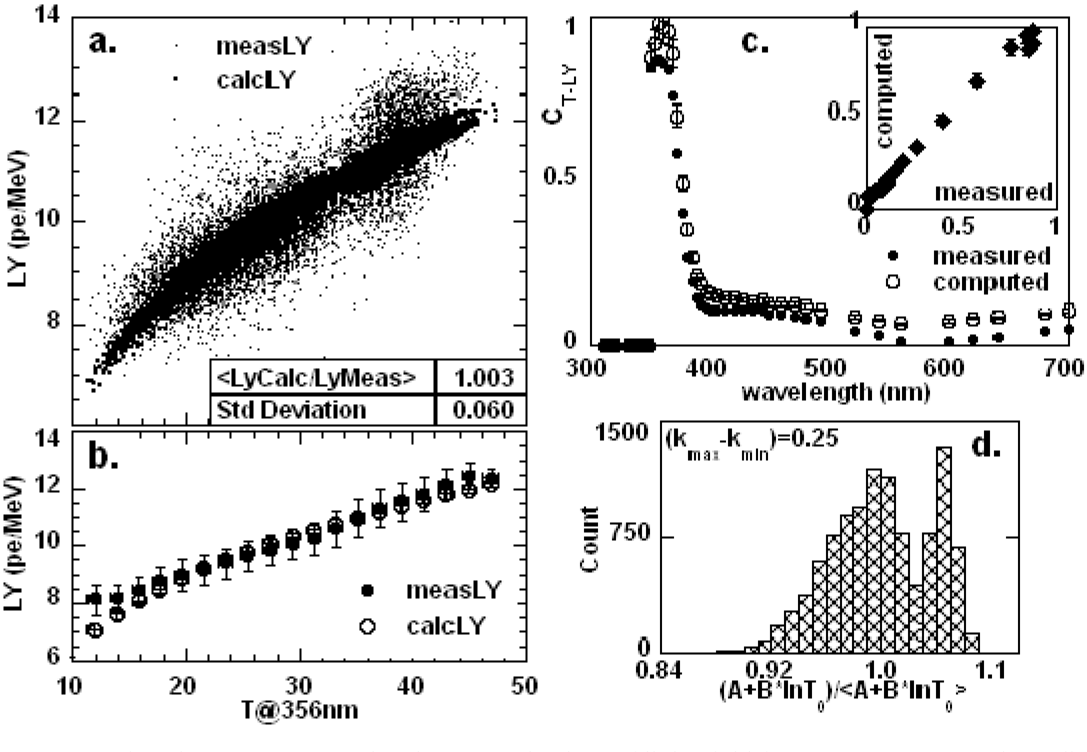

Figure 4: Comparison between measured and computed values of light yield for 11564 PWO crystals studied in this work: a) correlation between LT_{356} and measured and computed values of LY; b) LY- LT_{356} tendency curve ; c) measured and computed values of spectral correlation coefficient (correlation in inset); d) distribution of the coefficient $k=(A+B*lnT0)/< A+B*lnT0>$

The longitudinally measured transmission T at a given wavelength λ is given by [8]:

$$T_\lambda = \frac{t_\lambda^2 \cdot e^{-\alpha_\lambda \cdot L}}{1 - r_\lambda^2 \cdot e^{-2\alpha_\lambda \cdot L}} \qquad (6)$$

where L is the crystal length and r, t and α the reflectance, transmittance and absorption coefficient of the material respectively. Given the values of $r=0.004$ and $t=0.996$ [8], and the typical values for T in the region close to the absorption edge on PWO crystals $(0.25<T_0<0.55)$ one can approximate:

$$T_0 = t_0^2 \cdot e^{-\alpha_0 \cdot L} \qquad (7)$$

which allows for the calculation of the absorption coefficient and therefore the concentration of trapping centers concentration n_t :

$$n_t = a + n_b - b \cdot \ln T_0 \qquad (8)$$

where $a>0$, $b>0$ and n_b are parameters supposed to have the same value for all PWO crystals belonging to a same delivery batch (presumably produced in same conditions). Equation (3) becomes:

$$LY = (A + B \cdot \ln T_0) \cdot \int f(\lambda) \cdot \mathrm{T}^{\mathrm{n}}(\lambda) \cdot \varepsilon_{\mathrm{PM}}(\lambda)\, \mathrm{d}\lambda \qquad (9)$$

which allows for the calculation of the light yield of a given PWO crystal of known transmission spectrum $T(\lambda)$. The values of parameters n , A and B may be obtained by fitting measured and computed values of LY for a given batch of PWO crystals produced in the same conditions (same raw material, growth and post-growth procedures and same mechanical processing). The λ_0 value needed for T_0 values in (11) is previously chosen as the peak value of the spectral correlation coefficient (eq. 1) for the respective batch of crystals. In the present work the best fit was found minimizing the chi square of the difference between measured and calculated LY values:

$$\chi^2 = \frac{1}{\varepsilon_{\exp}^2} \cdot \sum_j (LY_j - LY_{j\exp})^2 \qquad (10)$$

with $\varepsilon_{exp}=0.49$ the value of experimental error of LY measured with ACCOR machine [9] in Rome.

4 Experimental data analysis

The results of the fitting procedure applied for the whole set of 11564 crystals are given in fig. 4. In spite of the simplicity of the model and of relative non-uniformity of crystals belonging to different batches coming from a production extended over several years, the mean value obtained for the ratio $LY_{computed}/LY_{measured}$ is 1.003 with a standard deviation of 0.06. As a consequence, the correlation between calculated LY values and measured T is similar to the one obtained for measured LY values as shown in fig. 4c. The proposed model allows also for an estimation of the spread of scintillation intensities among the set of analyzed crystals. For the group of 11564 crystals this estimation gives a 25% spread of scintillation intensities. A considerably improved coincidence between computed and measured LY values is obtained when the model is applied for a single batch of crystals (higher uniformity of crystals properties). Fig. 5 gives the synthesis of the results obtained for a single delivery batch (Batch #10).

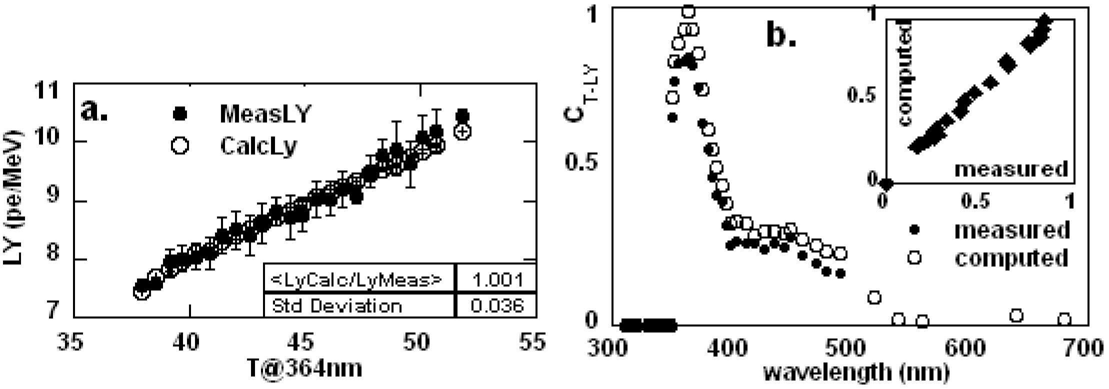

Figure 5: Comparison between measured and computed values of light yield for crystals of Batch #10: a) LY- T_{364} tendency curve; b) measured and computed values of spectral correlation coefficient (correlation in inset)

5 Conclusions

Statistical analysis of data stored in ECAL-CMS construction databases may give hints on scintillation characteristics of large PWO crystals, otherwise impossible to be put in evidence. The strong correlation noticed between *LY* and *T* in the absorption band edge region of PWO crystals is not driven by transparency variations from crystal to crystal. The semi-empirical model based on the assumption that scintillation intensity variations from crystal to crystal may exist, has an overall (11564 crystals) 6% guess precision, going to 4% for separate batches of crystals. In addition the model predicts an overall variation of light production efficiency in a range of 25% of the mean value for the 11564 crystals analyzed. The variation range may drop to 5% for uniform batches. Beyond the results on PWO crystals used for the construction of the Electromagnetic calorimeter of CMS, the work offers an analysis tool for large sets of scintillators, particularly interesting in the case where *LY* measurement cannot be made with sufficiently high precision and transmission measurement can bring the necessary improvement.

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