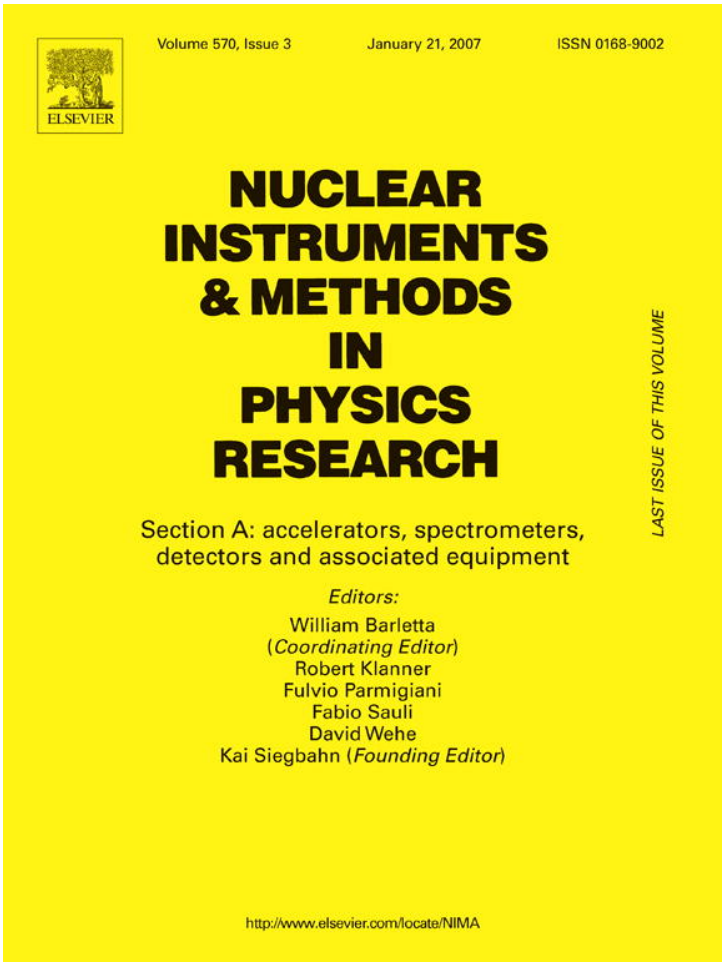

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The Monte-Carlo refractive index matching technique for determining the input parameters for simulation of the light collection in scintillating crystals

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Abstract

The Monte-Carlo refractive index matching (MCRIM) technique was developed to determine the physical properties of heavy inorganic scintillators (HIS) which are difficult to measure experimentally. It was designed as a method for obtaining input parameters for Monte-Carlo (MC) simulations of experimental arrangements incorporating HIS in their setups. The MCRIM technique is used to estimate the intrinsic light yield, the scattering coefficient and the absorption coefficient, herein referred to as indirect measurement properties. The MCRIM technique uses an experiment/MC combination to determine these indirect measurement properties. The MCRIM experimental setup comprises a crystal placed on a photomultiplier tube window with the possibility of introducing materials of different refractive indices in a small gap between the crystal and photomultiplier tube (PMT) window. The dependence of the measured light yield on the refractive index of the material in the gap can only be reproduced by simulations if the correct values of scattering, absorption and intrinsic light yield are used. The experimental setup is designed to minimise the presence of optical components such as unpolished surfaces and non-ideal reflectors, which are difficult to simulate. The MCRIM technique is tested on a $1.03 \times 1.00 \times 0.82\,cm^3$ crystal of $CaWO_4$ which is found to have a scattering coefficient of $0.061 \pm 0.005\,cm^{-1}$, an absorption coefficient of $0.065 \pm 0.005\,cm^{-1}$, and an intrinsic light yield of 22700 ± 1700 photons/MeV.

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Keywords: Inorganic scintillators; $CaWO_4$; Light yield; Monte-Carlo; Scattering coefficient

1. Introduction

Heavy inorganic scintillators (HIS) are increasingly being used for high-energy physics experiments such as the CMS [1], for medical physics [2] or for rare event searches [3]. For optimum detection efficiency, the scintillator material should have a high light yield combined with a high photon collection efficiency of the setup. The optimisation of the detection efficiency is usually carried out by trial and error plus experience acquired from previous work. Experimental optimisation procedures are expensive and time-consuming as they involve growing numerous crystals, research on after-growth treatment, processing, re-polishing and iterations on the geometry of the setup. Simulating the light collection properties by Monte-Carlo (MC) techniques would be a cheap and efficient alternative, but MC simulations of HIS still have to prove themselves as reliable tools. A survey of publications, which include comparisons of MC simulations and experiments containing HIS reveals recurrent discrepancies. MC simulations of HIS are difficult to perform, due to the following reasons:

(1) HIS have a high refractive index ($n > 1.8$), which causes a large proportion of photons to be trapped by total internal reflections. Surface properties and small geometrical inhomogeneities can have a significant effect on the proportion of trapped photons, affecting the measured light yield (MLY) of a given crystal.

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(2) HIS are often used with de-polished (lapped or roughened) faces and wrapped in reflectors. In general, simulations of realistic reflecting surfaces (for example, aluminium with a thin oxidised layer) and de-polished faces are difficult to perform [4–7].
(3) HIS crystals are often optically anisotropic. This adds the complication of the refractive index, absorption coefficient, and scattering coefficient depending on the direction of light propagation inside the crystal.
(4) HIS, as well as other solid-state scintillators can contain a non-negligible amount of lattice distortions, resulting from impurities or ion-deficient sites. This causes scattering, which needs to be accounted for when performing simulations and requires knowledge of the scattering coefficient, which is difficult to measure directly.

The approach which led to the development of the Monte-Carlo refractive index matching (MCRIM) technique was to concentrate on solving one of the problems, namely establishing the scattering coefficient. In order to be in a position to perform more complex simulations, a MC/experiment combination was devised which allows evaluating the amount of scattering in a crystal whilst minimising the impact of other difficulties. The experiment only contains a well-shaped, polished crystal and a photomultiplier tube (PMT). This eliminates uncertainties due to geometrical variations, de-polishing and reflectors.

The MCRIM technique was developed as part of a larger project on the optimisation of the light collection efficiency of $CaWO_4$ and $ZnWO_4$ crystals for dark matter searches. Since both crystals are birefringent it was necessary to select a MC program able to simulate optical anisotropy and the publicly available program Litrani [8] was chosen. Litrani was developed by the CMS group for the simulation of light transport in $PbWO_4$ [9]. It was mainly designed for use in high energy physics, and therefore C++ classes were added to simulate energy depositions of <1 MeV, taking into account effects of non-proportionality in light yield [10], Compton scattering [11] and photoelectric absorption of γ-rays [12]. The MCRIM technique uses this enhanced version of Litrani to reproduce the light yield measurements on a single crystal of $CaWO_4$.

2. Properties of the $CaWO_4$ crystal

The most important element of the experimental setup is the scintillating crystal. In order to perform a MC of light collection in a crystal, it is necessary to know its physical properties so that these can be used as input parameters. The physical properties of $CaWO_4$ can broadly be divided into two types: invariant properties and sample dependent properties. The invariant properties include the atomic mass ($A = 288$), the density ($\rho = 6.06\,g/cm^3$) and the cross-sections for interaction with γ-rays, which can be obtained from databases [12] (for the photoelectric effect) or calculated from first principles (for Compton scattering). The indirect measurement properties are all variable properties since their values depend on the presence of micro- and macroscopic defects, which vary according to the growth materials and treatment procedures. For the MC to be accurate, the sample dependent properties have to be measured for each crystal that will be simulated.

The crystal of $CaWO_4$ used in this work was grown from 4 N purity materials by SRC Carat (Lviv, Ukraine) using the Czochralskii technique. The dimensions of the crystal were $1.03 \times 1.00 \times 0.82\,cm^3$ and the surfaces received extra polishing using 0.25 μm diamond grit. The faces were checked to be plane and parallel to 2 μm using an interferoscope and an auto-collimated microscope. In the absence of impurities, $CaWO_4$ emission comes from a single Gaussian band centred at 430 nm with a FWHM of 50 nm [13]. The refractive index of $CaWO_4$ at maximum emission is $n_o = 1.96$ and $n_e = 1.98$ [14].

There are a further three parameters which cannot be measured directly (the indirect measurement properties). These parameters are the intrinsic light yield, the absorption and the scattering coefficients (respectively, the reciprocal of the absorption and scattering lengths).[1] The indirect measurement properties are also sample dependent as they depend on the presence of micro- and macroscopic defects produced during the growth and treatment processes.

The intrinsic light yield (N_0): The intrinsic light yield is defined as the number of photons produced per MeV of deposited energy as opposed to the number of photons per MeV that escape the crystal and are detected. The methods for determining N_0 in HIS can be generally divided into two categories. Firstly, there are relative measurements [15,16] used to determine N_0 by comparing the MLY with that of a scintillator of known properties such as NaI(Tl). The second possibility is to perform absolute measurements and to try to correct for light losses in order to obtain N_0 [17–19]. Previous measurements report the N_0 of $CaWO_4$ as being of the order of magnitude of ~10000 ph/MeV [20] with variance depending on the sample quality. It should be noted that this value is also dependent on the type of incoming radiation (γ-ray, α-particles, neutron) and the amount of energy deposited $N_0 = N_0(E_{dep})$, an effect known as the non-proportionality of light yield which has been studied in $CaWO_4$ by Moszyński et al. [21].

The absorption coefficient (α_{abs}) *and scattering coefficient* (α_{scat}): As mentioned above, these parameters cannot be measured independently. What can be measured is the attenuation coefficient α_{att}, which is related to the absorption α_{abs} and scattering α_{scat} by Eq. (1).

$$\alpha_{att} = \alpha_{scat} + \alpha_{abs}. \quad (1)$$

Measuring α_{att} reduces the number of unknown parameters from two (α_{scat}, α_{abs}) to one (i.e. if α_{att} and α_{scat} are known,

[1] It should be noted that one can measure the attenuation coefficient (sum of the absorption and scattering coefficients) via transmissivity measurements for example.

α_{abs} is also known). The problem can be reorganised by introducing a ratio of scattering to absorption coefficients B [22,23]:

$$B = \frac{\alpha_{scat}}{\alpha_{abs}}. \quad (2)$$

The higher the value of B, the more scattering occurs inside the crystal (for constant α_{att}). Since α_{abs} and α_{scat} are completely defined in terms of α_{att} and B, there are only two unknown parameters necessary for performing simulation: N_0 and B.

3. Principles of the MCRIM technique

The MLY of a scintillator is defined by the product of the intrinsic light yield (N_0) and the light collection efficiency of the setup in which the crystal is placed (η). In general, η is dependent on a number of parameters such as the geometry of the crystal and the setup, as well as the optical properties of the materials used in the experiment.

$$\text{MLY} = N_0\eta(\text{optical properties, geometry}\ldots). \quad (3)$$

For MC simulations to accurately predict the MLY of a setup, all parameters, including N_0 and B need to be known. The latter cannot be measured directly and therefore the problem is reversed: "How can simple experimental measurements and MC simulations be used to extract the values of B and N_0"? As the MLY is dependent both on N_0 and B, it is clear that a single measurement cannot determine both quantities. By taking the ratio of the MLY in two distinct experiments, the dependence on N_0 can be eliminated:

$$R_{1/2} = \frac{\text{MLY}_1}{\text{MLY}_2} = \frac{\eta_1}{\eta_2}. \quad (4)$$

The experimental quantity of interest is $R_{1/2}$, the ratio of MLY between experiments 1 and 2. For $R_{1/2}$ to be a useful quantity, experiments 1 and 2 must obey the following conditions: firstly, the same crystal must be used in order to ensure that N_0 is constant. Secondly, the number of parameters that change between the two experiments should be kept to a minimum so that changes to η are well understood. This excludes using geometrical variations by cutting crystals, as this influences surface properties at the same time as changing the geometry. Finally, experiments 1 and 2 must differ in such a way as to permit the determination of B (Fig. 1).

To find an appropriate set of experiments, a simple model of light propagation is considered. The most basic light yield measuring experiment is a crystal placed on a PMT window of the same area as the crystal face. Scintillation light is produced at a point inside the crystal with an isotropic distribution. The fraction of light that exits the crystal in direction of the PMT (p) is defined

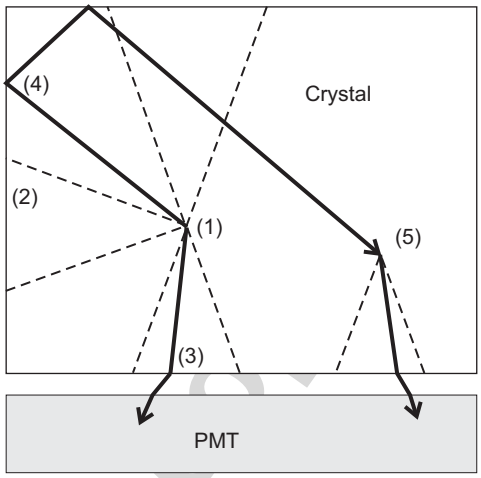

Fig. 1. Illustration of the possible fates for scintillation photons. (1) Point of interaction of radiation with crystal. (2) One of the six escape cones defined by Snell's law (only three are shown in the diagram). (3) A photon produced with a direction which falls inside an escape cone and is detected by the PMT. (4) A photon produced with a direction that falls outside of all escape cones undergoes total internal reflection at all faces. (5) A trapped photon undergoes scattering and is detected by the PMT.

by Snell's law:

$$\theta_C = \sin^{-1}\left(\frac{n_{air}}{n_{crystal}}\right)$$

$$p = \left(\frac{\tan(\theta_C)}{2}\right)^2. \quad (5)$$

Of the remaining light, a further $5p$ of the photons is lost by light exiting the crystal in a direction which leads away from the PMT window. In this approximation, there is a fraction $(1-6p)$ of photons, which remains "trapped" in the crystal. The trapped light can either be absorbed or scattered, the scattering probability is given by

$$S = [1 - \exp(-\alpha_{scat}d)] = [1 - \exp(-B)] \quad (6)$$

where d is the characteristic distance travelled by photons before being absorbed ($d = \alpha_{abs}^{-1}$). The fraction of observed light coming from this scattering (p') is given by the product of S, the amount of trapped light $(1-6p)$ and the fraction of light which can exit the crystal after isotropic scattering (p):

$$p' = p(1 - 6p)S. \quad (7)$$

Repeating the above steps for the remaining trapped light yields a geometrical series, which can be summed to produce an expression for the collection efficiency (η):

$$\eta = p + p(1 - 6p)S + p(1 - 6p)^2S^2 + \ldots = \frac{p}{[1 - (1 - 6p)S]}. \quad (8)$$

In such a way the collection efficiency of a simple experiment can be calculated. For example, in a crystal with $B = 0.1$, $n_{cryst} = 2.0$, surrounded by air, $\eta = 0.085$ according to the simple model. If $B = 1.0$, $\eta = 0.12$, i.e., an increase in scattering increases the MLY.

It is possible to consider a second similar setup using the same model. When a material of different refractive index is placed in between the face of the crystal facing the PMT and the PMT window, the expression for the collection efficiency must be modified to take into account that one face is in contact with a different material:

$$\eta = \frac{q}{[1-(1-5p-q)S]} \tag{9}$$

where q is the proportion of light which can escape from the side facing the PMT and is defined by replacing n_{air} by n_{gap} (refractive index of the gap material) in Eq. (5). Using the same example as before and $n_{gap} = 1.5$, $\eta_1 = 0.31$ for $B_1 = 0.1$; and $\eta_2 = 0.37$ for $B_2 = 1.0$ (PMT quantum efficiency is not included). The experiment with a material in between the crystal and the PMT can serve as the "ratio experiment" to eliminate the dependence on N_0 and to be able to compare experimental measurements with simulations. It requires no change of crystal, it is easy to perform experimentally and there is only one variable parameter (n_{gap}). Taking the cases of $B_1 = 0.1$ and $B_2 = 1.0$, $R_{1/2}$ is found to be 27% and 33%, respectively, indicating that the value of $R_{1/2}$ can therefore also provide information on B. Fig. 2 shows how $R_{1/2}$ is expected to depend on B in the range $0.01 < B < 10.0$.

MC simulations which iterate on the value of B can be used to match the values of $R_{1/2}$ between the experiment and simulations. This is the basis of the MCRIM technique. Knowing B, the collection efficiency for any of the performed experiments can be determined, and it is possible to work backwards to obtain N_0 for the crystal that is being measured using Eq. (3). Thus, in conjunction with transmissivity measurements, the MCRIM technique can be used to determine the indirect measurement properties of a crystal. The following section presents the experiments used to test the MCRIM technique on a crystal of $CaWO_4$.

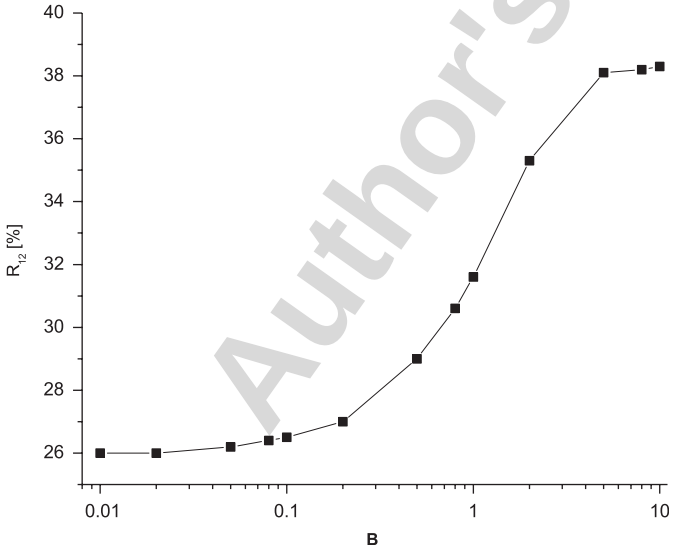

Fig. 2. Predicted dependence of $R_{1/2}$ on the ratio of scattering to absorption coefficients B. Experiment (1) is a $CaWO_4$ crystal surrounded by air, experiment (2) has a material with $n = 1.5$ in between the crystal and the PMT.

4. Experimental

4.1. Attenuation coefficient and light yield experiments

To determine the attenuation coefficient, the reference $CaWO_4$ crystal was placed in a Perkin-Elmer Lambda 15 UV/VS spectrophotometer, which can measure transmissivity in the range 200–800 nm. Special attention was given to possible contributions from surface effects such that uncertainty on the attenuation coefficient was reduced to 20%. The attenuation coefficient measured for the sample of $CaWO_4$ used for the MCRIM measurements is $\alpha_{att} = 0.126 \pm 0.025\,cm^{-1}$.

Once the attenuation coefficient has been measured, the crystal is placed into the MCRIM setup (see Fig. 3). The setup has been designed to exclude components, which MC simulations have problems reproducing, i.e., unpolished surfaces, uneven optical contacts and reflectors. The aim is to have an experiment comprising only a source, a well-shaped crystal and a PMT. To eliminate the need to simulate reflecting surfaces, all components that are not optically necessary (PMT shielding, light tight box, source holder) are painted black so that incident light is absorbed. The light tight box in which the PMT and crystal are placed is made large compared to the size of the crystal, making the chance of reflections from these sides back to the PMT window negligible. This means that photons, which exit the crystal and are not travelling toward the PMT are not detected. Similarly, all unpolished surfaces have been eliminated. The crystal is placed onto the window of an Electron Tubes 9125B PMT and the photoelectrons created by scintillation light are read out in photon counting mode using electronics and software from the multi-photon coincidence counting (MPCC)

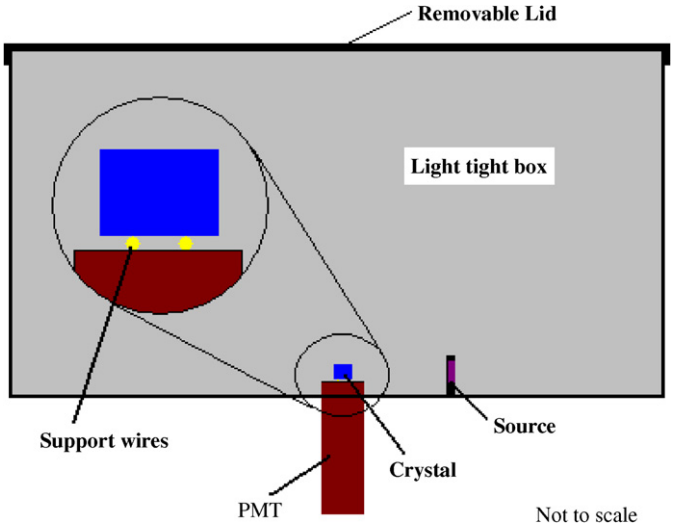

Fig. 3. Schematic drawing of the experimental setup. The crystal size is $1.03 \times 1.00 \times 0.82\,cm^3$ and the size of the box is $40 \times 40 \times 20\,cm^3$.

method [24]. The MPCC technique allows for accurate photon counting in "slow" scintillators such as $CaWO_4$. The MPCC electronics was modified by removing one PMT, giving up the coincidence condition. A self-trigger signal was used instead while spurious events were removed using offline software. A 59.5 keV γ-ray source (^{241}Am) is placed at a horizontal distance of 5 cm from the crystal.

To ensure that the gap between the PMT window and the crystal is well defined, supporting wires of thickness 0.05 mm are introduced between the crystal and PMT window. There is therefore a well-defined gap of constant thickness between the crystal and the PMT window, which can be filled by various transparent materials. Choosing the filling material is equivalent to controlling the refractive index of the gap (n_{gap}). During the MCRIM measurements, three fillers were used: air ($n_{gap} = 1.0$), Thorlabs G608N gel ($n_{gap} = 1.46$) and water ($n_{gap} = 1.34$). Care has to be taken to ensure that the amount of gel or water present completely fills the crystal–PMT gap, but no more. Studies demonstrated that a failure to consider the presence of excess or shortage of material can lead to discrepancies of up to 30% in MLY.

4.2. MC simulation

The properties of $CaWO_4$ in the MC are taken from the measurements of Section 4.1. The borosilicate PMT window is simulated as having a refractive index of 1.47. The gap between the crystal and the PMT window has the same surface area as the bottom face of the crystal and thickness 0.05 mm. Depending on the material present in the gap, the refractive index of the gap is entered as 1.0 (air), 1.34 (water) or 1.46 (gel). The undetermined input parameters N_0 and B are variables to be defined for each simulation run.

Before testing the MCRIM technique, studies were performed to verify that the attenuation length was known with sufficient precision for a meaningful prediction of the MLY. MC studies showed that the MLY would only vary by 1% even if α_{att} varies by 20%, meaning that α_{att} has been measured with sufficient precision for the purpose of the MCRIM technique.

5. Results and discussion

Fig. 4 shows a histogram of the number of photons measured per event when the gap is filled by air. The MLY due to ^{241}Am γ-rays (59.5 keV) is 51.5 photoelectrons (p.e.). Table 1 shows the results of light yield measurements when the gap is filled with air, water or gel.

The values and errors are calculated from the repetition of three measurements. The analysis which forms the basis of the MCRIM technique only requires the measurement of the MLY using air and gel. The ratio between the MLY of the experiments with the gap filled by air and gel is $R_{air/gel} = 46.9 \pm 0.7\%$. As already stated, this value is independent of the intrinsic light yield of the crystal and

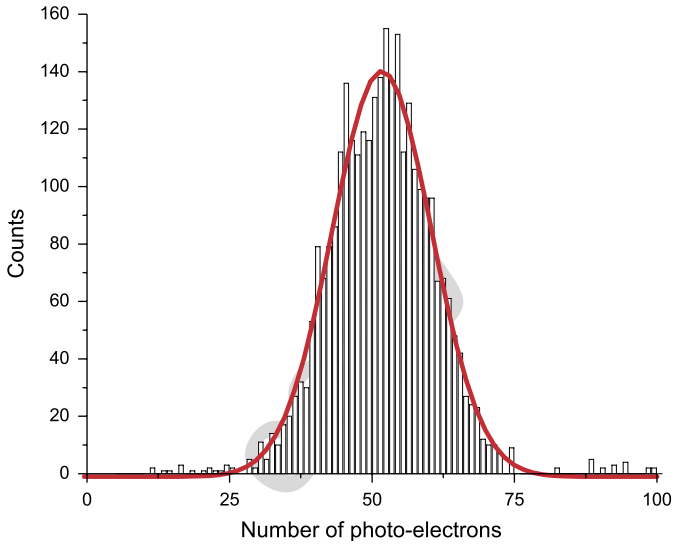

Fig. 4. Spectrum of ^{241}Am γ-rays in a $CaWO_4$ crystal obtained using a PMT in photon-counting mode. The data is fitted to a single Gaussian curve with a centre at 51.5 photoelectrons and a standard deviation of 8.5 photoelectrons.

Table 1
Results of light yield measurements for different materials placed in the gap between the PMT and crystal

Material in gap	n_{gap}	MLY (p.e.)
Air	1.0	51.5 ± 1.0
Water	1.34	94.3 ± 1.5
Gel	1.47	110 ± 1.0

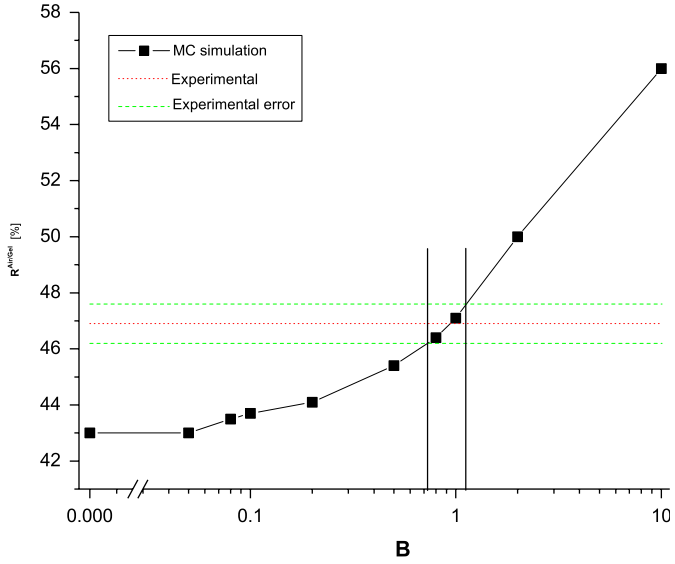

Fig. 5. Ratio of light yield with the gap filled once with air and once with gel ($R_{air/gel}$) vs. the ratio of scattering to absorption (B). The experimental value and associated error ($R_{air/gel} = 46.9 \pm 0.7\%$) are represented by the dashed lines. By comparison with the simulated values (points and solid line), it is found that B is situated in the range 0.73 to 1.13. The final estimate for B is the mean of this range: $B = 0.93 \pm 0.2$.

can be used to determine B. Fig. 5 shows $R_{air/gel}$ calculated as a function of B using MC simulations.

By comparing the results of the simulations with the measured $R_{air/gel}$, a value of B can be inferred. In Fig. 5, B can be extracted by comparing where the simulation curve (solid line) intersects the experimental value of $R_{air/gel}$ (dotted line). The error on B (vertical lines) is evaluated by considering where the simulation curve intersects the experimental error lines (dashed lines). This places B in a range from 0.73 to 1.13. The best value for B is given by taking the mean between the two vertical lines which corresponds to $B = 0.93 \pm 0.2$. Since $\alpha_{att} = 0.126 \pm 0.025\,cm^{-1}$, the scattering and absorption coefficients can be calculated as $\alpha_{scat} = 0.061 \pm 0.017\,cm^{-1}$ and $\alpha_{abs} = 0.065 \pm 0.018\,cm^{-1}$.

Having determined B, the collection efficiency can be calculated by MC, and using Eq. (3) it is possible to deduce the intrinsic light yield. The values of B are chosen to cover the uncertainty on B, i.e. $B = 0.73$ and 1.13. Once the collection efficiency has been calculated, N_0 is deduced by requiring the simulated light yield to match the MLY of the experiment. Table 2 shows the figures used for N_0 from the measurements when air is present in the PMT-crystal gap.

To find the errors on N_0, simulations were carried out using the limits of B as input parameters. This provides the range of collection efficiencies which is used to derive the range of intrinsic light yield. The best estimate of the intrinsic light yield is taken as the mean of the extreme values: $N_0 = 22700 \pm 1100$ ph/MeV (note: the error on N_0 does not represent the width of the intrinsic light yield distribution but is the uncertainty on the peak position). This completes the steps of the MCRIM technique. The scattering to absorption ratio and the intrinsic light yield have been calculated and all the properties of the reference crystal of $CaWO_4$ needed for simulations are now determined.

Table 2
Values used to fix N_0 using the MCRIM technique

B	η (%)	N_0 (ph/MeV) at 59.5 keV	Simulated MLY (p.e.)
0.73	3.64	23,800	51.5
1.13	4.01	21,600	51.5

The values of B are chosen to represent the range 0.93 ± 0.2 which fixes the collection efficiency. The value of N_0 is then tuned so that the simulated MLY is equivalent to the one observed in the experiment.

6. Tests of the MCRIM technique

The measurements performed with water in the PMT-crystal gap were used as a test of the MCRIM performance. Using the calculated values of B and N_0, the light yield of the experiment with water filling the gap was predicted as 93.9 photoelectrons. This is in good agreement with the measured value of 94.3 ± 1.5. Given the difficulties of performing simulations of HIS, this is a good indication of the power of the MCRIM technique. It should be stressed that an accurate prediction of the MLY could not have been obtained without considering scattering effects or without using the correct value of N_0.

A further test of the technique was carried out by simulating the results from a published experiment [21] using the indirect measurement properties determined by MCRIM. The experiment was selected as it contained a crystal cut from the same ingot as the reference crystal described above, i.e., with the same intrinsic light yield and scattering and absorption coefficients. The setup comprises a PMT of characteristics similar to those of XP2020Q and the crystal has dimensions $1.0 \times 1.0 \times 0.8\,cm^3$. The crystal is irradiated by a ^{137}Cs γ-ray source, and the input intrinsic light yield is corrected for non-proportionality effects. Results reported in the same paper [21] indicate that the light yield at 59.5 keV is approximately 95% of that at 662 keV, hence the intrinsic light yield as predicted by the MCRIM technique at 662 keV is $N_0 = 24000$ ph/MeV. The crystal in the experiment is wrapped in Teflon tape, which is simulated by a 99% reflective surface. The tape is deliberately chosen as being highly reflective for reasons explained below. Of the reflected photons, 95% are reflected diffusely, 5% through specular reflections. It was shown that the exact proportion has little effect of the light yield as long as the amount reflected diffusely is much larger than the amount undergoing specular reflection.

The results of the experiment and predicted MLY of the MC are shown in Table 3. The MLY is 4400 ph/MeV whilst the predicted MLY is 3900 ph/MeV, i.e. a 10% discrepancy. The lack of agreement can be explained by considering that the crystal in Moszyński et al. [21] has not undergone shaping and polishing treatment to ensure that it can be accurately simulated by MC. This results in a reduced proportion of trapped photons, increasing the MLY in ways, which cannot be reproduced by the MC.

The fourth column of the table shows the value of N_0 deduced by using the standard technique of comparing the MLY of $CaWO_4$ to that of an NaI(Tl) in the same setup.

Table 3
Comparison of predicted and measured MLY for a published experiment [19]

	MLY (p.e./MeV)	Input N_0 (ph/MeV)	N_0 relative to NaI(Tl) (ph/MeV)
Experiment	4400 ± 200	n/a	14,200
Prediction	3900	24,000	12,600

The last column is the light yield which is calculated by comparing the light yield of $CaWO_4$ with that of NaI(Tl).

The intrinsic light yield calculated using the comparative method is approximately 40% lower than that obtained using the MCRIM technique. This is attributed to the fact that the intrinsic light yield of NaI(Tl) has not been calculated using full corrections for scattering, photon trapping, Fresnel reflections and all other factors which can be accounted for by MC simulations. The MCRIM technique takes all these into account.

7. Conclusions

Simulating light collection in HIS has always been difficult due to the problems of obtaining good input parameters. In particular, evaluating the intrinsic light yield of HIS proves difficult due to their high refractive index. To complicate matters further, the light collection efficiency is dependent on the sample quality [25,26] and in particular on the scattering present in the crystal. It is shown in this paper that a higher scattering coefficient leads to higher light collection efficiency. A consequence of this is that simulating light transport in scattering crystals requires evaluation of α_{scat}. A new method has been developed to determine these parameters in HIS, called the MCRIM. The MCRIM method uses a combination of MC simulations and experimental measurements to determine the ratio of scattering to absorption coefficients (B) and the intrinsic light yield (N_0). A minimalist experimental setup is used which is designed to eliminate uncertainties due to reflectors, uneven and de-polished surfaces. A small, well-polished and regularly shaped crystal is placed on a PMT such that a small gap of controlled thickness is left between the bottom crystal face and the PMT window. Introducing transparent materials of different refractive index in the gap causes a change in the MLY, which can only be reproduced by simulations which have a unique set of B and N_0 as input parameters. The MCRIM technique was tested on a $1.03 \times 1.00 \times 0.82\,cm^3$ $CaWO_4$ crystal and the best estimate of its intrinsic light yield is $N_0 = 22700 \pm 1100$, and $B = 0.93 \pm 0.2$ that translates into absorption coefficients of $\alpha_{scat} = 0.061 \pm 0.017\,cm^{-1}$ and $\alpha_{abs} = 0.065 \pm 0.018\,cm^{-1}$, respectively. In the MCRIM reference crystal, scattering and absorption play approximately equal roles in attenuation processes.

The MCRIM technique was demonstrated to predict the MLY in an experiment where the crystal-PMT gap was filled with water. The fact that MC simulations can be used to predict the light yield of experiments indicates that the parameters calculated using the MCRIM technique are accurate. Furthermore, the ability to successfully calculate the MLY of crystals subjected to radiation is a stringent test on the exactitude of a MC simulation. It has been demonstrated that the Litrani code fulfils the prediction requirement under the condition that reflectors and de-polished surfaces are not included. It also gave a prediction accurate to 10% of a published experiment with a crystal for which knowledge of the quality of polish and shaping of the faces is incomplete. The reason that the prediction is not more accurate is probably due to these differences.

It has also been shown that traditional methods of evaluating the intrinsic light yield of HIS result in essential underestimation of N_0. The MCRIM technique is simple enough to be adapted to measure the scattering, absorption and intrinsic light yield for a range of crystal shapes and sizes, making it a promising tool for the optimisation of scintillation setups for a much wider range of applications including medical physics. Furthermore, the MCRIM technique increases the reliability of predictions for setups containing crystals of shapes and sizes that cannot easily be optimised by physical experiments due to time or cost constraints.

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