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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 $1.03 \times 1.00 \times 0.82\,\text{cm}^3$ crystal of $CaWO_4$ which is found to have a scattering coefficient of $0.061 \pm 0.005\,\text{cm}^{-1}$, an absorption coefficient of $0.065 \pm 0.005\,\text{cm}^{-1}$, and an intrinsic light yield of 22700 ± 1700 photons/MeV.

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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 ($\rho = 6.06\,\mathrm{g/cm^3}$) 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 $1.03 \times 1.00 \times 0.82\,\mathrm{cm^3}$ and the surfaces received extra polishing using $0.25\,\mu\mathrm{m}$ diamond grit. The faces were checked to be plane and parallel to $2\,\mu\mathrm{m}$ 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 $\sim$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 $N_0 = N_0(E_{\mathrm{dep}})$, 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).

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

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,

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