



# The Influence of Geometric Factors of CLYC-6 Crystal on Detection Efficiency and Luminous Efficiency

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## Abstract

Monte Carlo software MCNPX was used to simulate the influence of geometric factors and doping concentration of CLYC-6 scintillator detector on detection efficiency and luminous efficiency. It is found that with the increase of CLYC-6 crystal size, the detection efficiency increases nonlinearly, while the luminous efficiency decreases nonlinearly, and the changing trend of both decreases with the increase of crystal size. Under different particle radiation energies, the thickness of the CLYC-6 crystal is 2.54 cm, the bottom diameter is 17.78 cm, and the doping concentration ( $Ce^{3+}$ ) is 0.5%. The luminescence efficiency reaches the maximum value, and it has good detection efficiency. This result can provide a reference for the development of the CLYC-6 detector.

## Subject Areas

Nuclear Physics

## Keywords

Detection Efficiency, Luminescence Efficiency, Monte Carlo, CLYC Crystal

## 1. Introduction

$Cs_2LiYCl_6:Ce^{3+}$  (CLYC) is a new inorganic scintillator discovered in recent years, which has an excellent performance in neutron and gamma recognition measurement [1]-[5]. As a gamma ray detector, the CLYC scintillator has good energy resolution (less than 4% at 662 KeV gamma ray energy) and high light output, which is superior to the commonly used NaI (Tl) and CsI (Tl) detectors [6]. The CLYC scintillator rich in isotope  ${}^6Li$  can detect thermal neutrons through the reaction of  ${}^6Li$  (n, t) with a cross-section of 940 b, and its efficiency is equivalent to that of

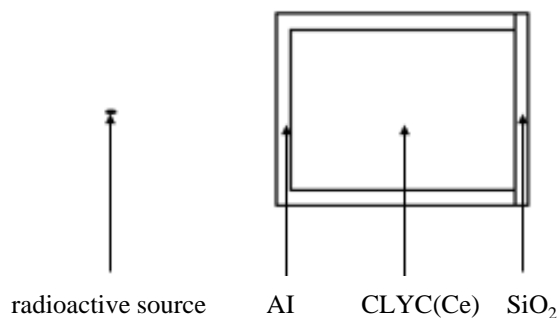
$^3\text{He}$  tube of similar size. The halogen-containing Cl in CLYC scintillator can detect the fast neutrons through the  $^{35}\text{Cl} (n, p)^{35}\text{S}$  reaction with a cross-section of about 0.1b [7] [8]. Due to the different attenuation times and amplitude (CVL) of the light signal component between charged particles (secondary particles produced in the neutron-induced reaction) and gamma rays, pulse shape recognition (PSD) can be used to distinguish neutron and gamma rays. These comprehensive properties make the CLYC scintillator widely used in experimental nuclear physics, particle physics, astrophysics and other fields.

In this paper, the effects of geometric factors and doping concentration ( $\text{Ce}^{3+}$ ) of CLYC-6 scintillator detector on the detection efficiency and luminous efficiency of CLYC-6 scintillator detector under  $\gamma$ -ray, thermal neutron and fast neutron irradiation was MCNPX program. This result can be used for relevant experimental research and detection.

## 2. Model Construction

MC method can realistically describe the characteristics and physical experiment process of things with random properties, which is mainly used in photon detection efficiency, neutron detection efficiency, flux and reaction rate [8] [9]. The MCNP program is a general program based on the MC method for calculating the transport problems of photons, neutrons, electrons or coupled photons, coupled neutrons and coupled electrons in three-dimensional complex geometric structures [10]. It is widely used by scientific researchers because of its problem solving, practical compliance and high accuracy.

The MC model of the CLYC-6 scintillator detector is shown in **Figure 1**, including scintillation crystal, photoconductivity and cladding layer, without considering the devices such as the photomultiplier tube. The radiation source is the point source, the energy of the gamma point source is 0.661 MeV, the energy of the thermal neutron point source is 0.225 MeV, and the energy of the fast neutron point source is 1 MeV. The distance from the probe surface is 5 cm, and the number of simulated particles is 10 million. Scintillation crystal shape is cylindrical, size change design as shown in **Table 1**, bottom diameter is 1 in - 7 in, and thickness is 1 in - 7 in before simulation has been transformed into the standard unit (cm). The front and side of the scintillation crystal are wrapped with a layer of 0.2 cm Al, and the back is 0.2 cm  $\text{SiO}_2$  optical glass.



**Figure 1.** MC model of CLYC-6 scintillator detector.

**Table 1.** CLYC-6 scintillator detector geometry size change table.

Crystal diameter/cm	2.54	5.08	7.62	10.16	12.7	15.24	17.78
crystal thickness/cm	2.54	5.08	7.62	10.16	12.7	15.24	17.78

### 3. Theoretical Basis

#### 3.1. Working Principle of CLYC Scintillator Detector

CLYC scintillator is based on the nuclear reaction method to measure neutron. The main reaction channels of thermal neutrons (0.025 eV) and fast neutron (>105 eV) detected by the CLYC scintillator are  ${}^6\text{Li}$  (n, t) a reaction and  ${}^{35}\text{Cl}$  (n, p) 35S reaction, respectively. The specific reaction channels are shown in Equations (1) and (2). The secondary charged particles generated by the nuclear reaction of neutron entering the scintillator lose energy in the scintillator and cause the scintillator luminescence.



The interaction between  $\gamma$ -ray and CLYC scintillator mainly loses energy through the photoelectric effect, Compton effect and electron pair effect [11]. CLYC scintillator under  $\gamma$ -ray irradiation can induce Core-to-Valence Luminescence-CVL (Core-to-Valence Luminescence-CVL) with attenuation time of about several ns between 220 - 320 nm light waves; this mechanism does not exist between neutron and scintillator. This makes the neutron and gamma rays in the CLYC scintillator will cause different pulse shapes, so the neutron and gamma can be separated by the pulse shape discrimination (PSD) method, which is also the basis for the application of CLYC scintillator detectors.

#### 3.2. Detection Efficiency and Luminous Efficiency

The luminous efficiency indicates the ability of the scintillator to transform the absorbed ray energy into a light pulse [12]. The higher the photon yield of the scintillator is, the more photons converge to the photoelectric equipment, and the higher the energy resolution is, and the better the performance of the scintillator is. (Absolute) luminous efficiency is defined as the ratio of the number of photons produced in the scintillation process to the energy loss of particles in the scintillator [13]. The expression is:

$$Y_{ph} = n_{ph} / \Delta E \quad (3)$$

In Formula (3),  $Y_{ph}$  is the luminous efficiency, unit  $\text{MeV}^{-1}$ .  $n_{ph}$  is the total number of photons generated in the scintillation body.  $\Delta E$  is the energy lost by incident rays or particles in the scintillation body, in MeV. Here, the F1 card in MCNPX program is used to record the optical integral flow on the left side of the photoconductor, namely (absolute) luminous efficiency.

The scintillator detector detects neutrons and gamma rays using the detection efficiency of  $\varepsilon_s$  source for calibration. The secondary particles generated by

gamma rays or neutrons interact with crystals to produce photoelectrons, which are collected by photocathodes and output electrical signal pulses through photoelectric conversion devices.  $\varepsilon_s$  source detection efficiency, also known as absolute detection efficiency, is defined as the ratio of the number of pulses generated by the interaction of rays and scintillators to the number of incident particles [14] [15]. The expression is:

$$\varepsilon_s = S_i / N \quad (4)$$

In Formula (4),  $\varepsilon_s$  is the source detection efficiency;  $S_i$  is the number of pulses or particles recorded;  $N$  is the number of particles emitted by the radioactive source. Here, the F8 card in the MCNPX program is used to record the pulse height spectrum of  $\gamma$ -ray in a scintillation crystal; E8 card is used to record the detection efficiency of the scintillation detector for  $\gamma$ -ray; the F4 card and FM4 multiplier card are used to record the detection efficiency of thermal neutron (n, t) reaction and fast neutron (n, p) reaction.

## 4. Simulation Experiment

### 4.1. Effects of Geometric Factors on Detection Efficiency and Luminous Efficiency

The detection efficiency and luminous efficiency of the CLYC-6 scintillator with different bottom diameters, different thicknesses and different kinds of particle energy were simulated. **Figures 1-3** show the changes in detection efficiency and luminescence efficiency of the CLYC-6 scintillator under 0.661 MeV  $\gamma$ -ray, 0.025 MeV thermal neutron and 1 MeV fast neutron irradiation, respectively. It can be seen from **Table 2** and **Figure 3** that the detection efficiency gradually increases with the increase of CLYC scintillator size. When the bottom diameter of the CLYC scintillator is constant, the greater the thickness, the greater the detection efficiency. When the thickness of the CLYC scintillator is constant, the larger the bottom diameter, the greater the detection efficiency. But as the size increases, the growth trend of detection efficiency will gradually slow down. It can be seen from **Table 2** and **Figure 2** that the luminous efficiency decreases with the increase of the size of the CLYC scintillator. When the bottom diameter of the CLYC scintillator is constant, the luminous efficiency decreases with the increase of thickness. When the thickness of the CLYC scintillator is constant, the larger the bottom diameter, the greater the detection efficiency. In general, the influence of the CLYC scintillator geometry on the detection efficiency and luminescence efficiency of  $\gamma$ -rays, thermal neutrons and fast neutrons conforms to the same rule; that is, with the increase of CLYC scintillator size, the number of particles entering the scintillator to react increases and the detection efficiency will gradually increase. The photons generated by this process will deposit in the crystal with the increase of the crystal size and cannot pass to the other side of the photoconductivity, which will reduce the luminous efficiency with the increase of the size of the scintillator. It can be seen that the continuous improvement of crystal size does not bring sustained growth in detection efficiency and luminous efficiency.

**Table 2.** Influence of CLYC crystal geometry on detection efficiency and luminescence efficiency.

diameter/cm	thickness/cm	0.661 MeV $\gamma$ -ray		0.025 eV thermal neutron		1 MeV fast neutron	
		detection efficiency	luminous efficiency	detection efficiency	luminous efficiency	detection efficiency	luminous efficiency
2.54	2.54	0.014292	0.005905	0.009698	0.000657	0.000025	0.000030
	5.08	0.014322	0.002031	0.009844	0.000187	0.000035	0.000018
	7.62	0.014345	0.000757	0.009956	0.000077	0.000039	0.000009
	10.16	0.014364	0.000298	0.010048	0.000047	0.000041	0.000005
	12.7	0.014379	0.000126	0.010121	0.000033	0.000042	0.000002
	15.24	0.014392	0.000057	0.010178	0.000026	0.000043	0.000001
	17.78	0.014402	0.000028	0.010224	0.000000	0.000043	0.000000
5.08	2.54	0.050337	0.020166	0.034483	0.004777	0.000099	0.000172
	5.08	0.050379	0.007690	0.034704	0.001652	0.000143	0.000121
	7.62	0.050411	0.003106	0.034880	0.000702	0.000165	0.000072
	10.16	0.050443	0.001298	0.035014	0.000354	0.000176	0.000041
	12.7	0.050462	0.000561	0.035118	0.000196	0.000182	0.000023
	15.24	0.050482	0.000252	0.035205	0.000124	0.000186	0.000013
	17.78	0.050496	0.000118	0.035280	0.000085	0.000188	0.000001
7.62	2.54	0.095650	0.039837	0.066168	0.012492	0.000210	0.000449
	5.08	0.095696	0.016197	0.066423	0.005099	0.000314	0.000347
	7.62	0.095730	0.006919	0.066622	0.002398	0.000369	0.000234
	10.16	0.095761	0.003047	0.066779	0.001213	0.000399	0.000147
	12.7	0.095787	0.001373	0.066903	0.000664	0.000417	0.000091
	15.24	0.095809	0.000628	0.067000	0.000388	0.000427	0.000059
	17.78	0.095822	0.000289	0.067081	0.000245	0.000433	0.000038
10.16	2.54	0.140637	0.061538	0.098311	0.022389	0.000343	0.000812
	5.08	0.140684	0.026362	0.098585	0.010252	0.000525	0.000686
	7.62	0.140721	0.011683	0.098796	0.005126	0.000628	0.000491
	10.16	0.140753	0.005320	0.098961	0.002724	0.000688	0.000338
	12.7	0.140779	0.002460	0.099091	0.001549	0.000725	0.000219
	15.24	0.140798	0.001157	0.099183	0.000912	0.000747	0.000149
	17.78	0.140812	0.000553	0.099258	0.000542	0.000762	0.000097
12.7	2.54	0.180729	0.082929	0.127464	0.032856	0.000486	0.001225
	5.08	0.180777	0.037033	0.127733	0.013482	0.000761	0.001120
	7.62	0.180812	0.016944	0.127939	0.008617	0.000924	0.000826
	10.16	0.180842	0.007906	0.128102	0.004745	0.001024	0.000595
	12.7	0.180866	0.003735	0.128221	0.002746	0.001087	0.000403
	15.24	0.180885	0.001778	0.128312	0.001647	0.001128	0.000284
	17.78	0.180896	0.000867	0.128384	0.001014	0.001154	0.000196

Continued

	2.54	0.214993	0.102695	0.152595	0.043039	0.000632	0.001663
	5.08	0.215041	0.047445	0.152850	0.022759	0.001007	0.001584
	7.62	0.215075	0.022338	0.153044	0.012583	0.001239	0.001241
15.24	10.16	0.215108	0.010621	0.153195	0.007139	0.001388	0.000926
	12.7	0.215129	0.005128	0.153308	0.004229	0.001485	0.000653
	15.24	0.215146	0.002483	0.153393	0.002565	0.001549	0.000469
	17.78	0.215156	0.001208	0.153449	0.001591	0.001592	0.000322
	2.54	0.243715	0.120139	0.173907	0.052236	0.000774	0.002102
	5.08	0.243758	0.057208	0.174154	0.029001	0.001254	0.002104
	7.62	0.243792	0.027549	0.174338	0.016588	0.001562	0.001708
17.78	10.16	0.243820	0.013336	0.174478	0.009684	0.001766	0.001303
	12.7	0.243839	0.006520	0.174581	0.005848	0.001902	0.000952
	15.24	0.243854	0.003217	0.174656	0.003565	0.001996	0.000689
	17.78	0.243865	0.001590	0.174701	0.002254	0.002059	0.000497

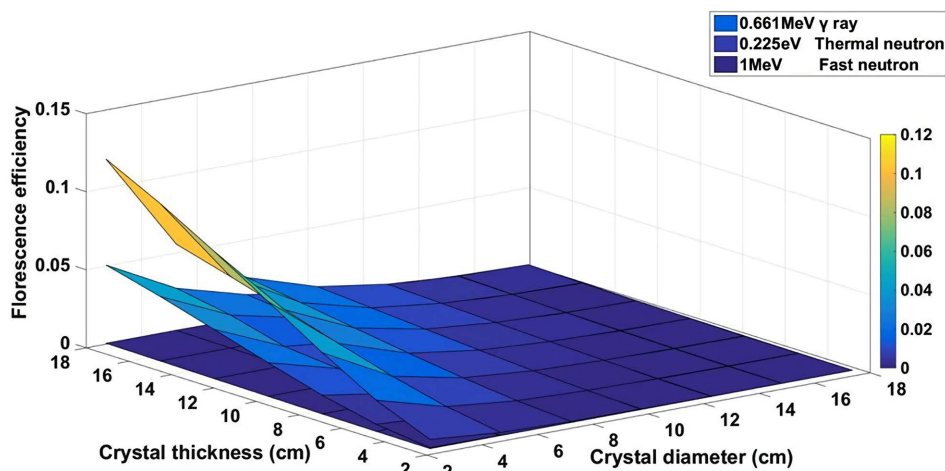


Figure 2. Relationship between geometrical factors and luminous efficiency of CLYC crystal.

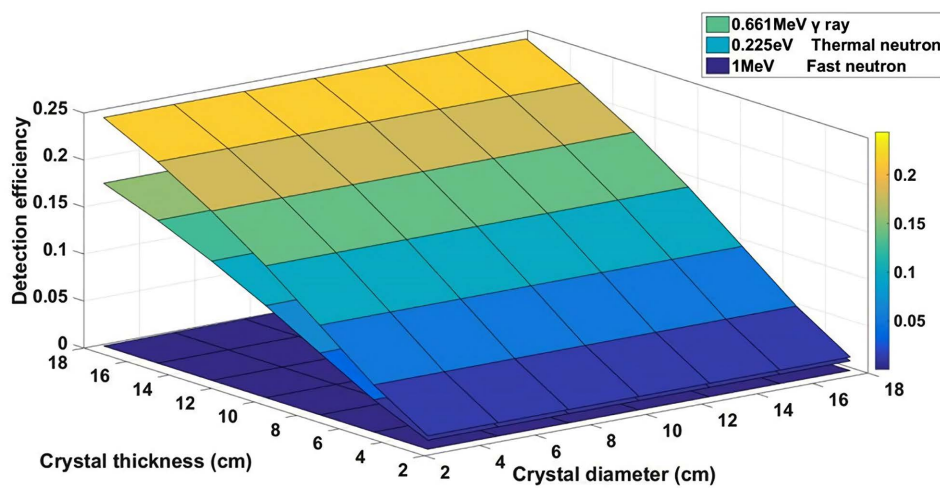


Figure 3. Relationship between geometrical factors and detection efficiency of CLYC crystal.

## 4.2. Effect of Ce<sup>3+</sup> Ion Doping Concentration on Detection Efficiency and Luminescence Efficiency of Scintillator

Ce<sup>3+</sup> ion, as the luminescent center of the CLYC scintillation crystal, plays a key role in the performance of the crystal and detector. The appropriate doping concentration can maximize the performance of the crystal. The influence of Ce<sup>3+</sup> ion doping concentration on the detection efficiency and luminous efficiency of the CLYC-6 scintillator with the size of  $\Phi 2.54 \text{ cm} \times 17.78 \text{ cm}$  was simulated. The incident particle is 0.661 MeV energy gamma-ray, and the Ce<sup>3+</sup> ion doping concentration is 0.1% - 1.0%. The simulation results are shown in **Table 3**. Ce<sup>3+</sup> ion doping concentration has no effect on the detection efficiency of the CLYC-6 scintillator, and the luminous efficiency reaches the maximum when the doping concentration is 0.50%.

## 4.3. Discussion

From **Tables 1-3**, the detection efficiency and luminous efficiency of the CLYC detector are affected by the geometric factors of CLYC crystal, doping concentration and source distance. When the CLYC detector detects three different single source particles, the changing trend of detection efficiency and luminous efficiency is similar. The detection efficiency increases with the increase of CLYC crystal size, and the luminous efficiency decreases with the increase of CLYC crystal size. It can be seen that the CLYC detector is not the bigger, the better. The CLYC-6 detector is rich in <sup>6</sup>Li, and the detection efficiency of thermal neutrons is nearly three orders of magnitude higher than that of fast neutrons. The CLYC-7 detector (containing <sup>7</sup>Li up to 99.9%) can be selected for fast neutron measurement. The CLYC-6 scintillator detector has the optimal luminous efficiency and excellent luminous efficiency when the size is  $\Phi 2.54 \text{ cm} \times 17.78 \text{ cm}$  and the doping concentration is 0.50%.

**Table 3.** Effect of Ce<sup>3+</sup> ion doping concentration on scintillator detection efficiency and luminescence efficiency.

doping concentration	detection efficiency	luminous efficiency
0.10%	0.243715	0.120109
0.20%	0.243715	0.120082
0.30%	0.243715	0.120051
0.40%	0.243715	0.120021
0.50%	0.243715	0.120125
0.60%	0.243715	0.119959
0.70%	0.243715	0.119920
0.80%	0.243715	0.119887
0.90%	0.243715	0.119862
1.00%	0.243715	0.119827

## 5. Conclusion

Monte Carlo software MCNPX simulation shows that the detection efficiency and luminous efficiency of the CLYC-6 scintillator detector are affected by geometric factors and doping concentration. The detection efficiency increases non-linearly with the increase of crystal size, and the luminous efficiency decreases with the increase of crystal size. These two trends will gradually slow down with the increase in crystal size. Increasing the crystal size does not bring the continuous benefits of detection efficiency and luminous efficiency. When the crystal is too large, the photons generated by the depolarization caused by the direct interaction between the incident particles and the crystal atoms or the secondary particles cannot escape from the scintillator, and the energy deposition causes the self-absorption effect, which cannot be transmitted to the photocathode to emit photoelectrons, resulting in the decrease of luminous efficiency. The influence of geometric factors and doping concentration of CLYC detector on detection efficiency and luminous efficiency studied in this paper can provide a certain reference for the development and application of CLYC detector.

## Conflicts of Interest

The authors declare no conflicts of interest.

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