

COMPUTATIONAL INVESTIGATION ON ALPHA, PROTON, NEUTRON, AND GAMMA-RAY INTERACTION OF LaCl₃:Yb CRYSTAL

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Abstract

This study investigated the interaction of alpha, proton, neutron, and gamma with LaCl₃:Yb crystal. These interaction of the LaCl₃:Yb crystal were calculated by approaches using TRIM/SRIM code, WinXCom program and Monte Carlo simulation. The parameters, including the total atomic cross-section ($\sigma_{t,a}$), effective atomic number (Z_{eff}), effective electron density (N_{eff}), half-value layer (HVL), mean free path (MFP), total mass stopping power (TMSP) and projected range (PR) are shown graphically with energy function. The simulation results show that the photon interaction parameters obtained by FLUKA and WinXCom programs are in good agreement. The results revealed that the variation of these parameters was changed with energy. The obtained results suggest using these crystal samples for various photon charged particle and neutron detection applications.

Keywords: LaCl₃:Yb crystal; Monte Carlo simulation; Radiation shielding; SRIM code; WinXCom

Introduction

Nowadays, the use of ionizing radiation is prevalent in several domains, such as food irradiation, medical imaging, radiation treatment, and other related disciplines. Nevertheless, the potential hazards associated with ionizing radiation remain a topic of concern due to its ability to induce ionization in matter. Therefore, the detection and spectroscopy of radiation play a crucial role in security checks to avoid unwanted radiation hazards. To attain this purpose, researchers have

investigated scintillation materials that possess the ability to convert radiation into visible light. These materials have been developed with different compositions to improve their performance. In the last several decades, a considerable amount of study has been accomplished on halides single crystals, including LaCl₃:Ce³⁺ (Andriessen *et al.*, 2000; McIntyre *et al.*, 2011), LaBr₃:Ce³⁺ (Van Loef *et al.*, 2002; Glodo *et al.*, 2005), LaBr₃:Sm²⁺ co-doping of Ce³⁺ or Pr³⁺ (Van Aarle *et al.*, 2023). The LaCl₃

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(lanthanum chloride) single crystal is a scintillation crystal, which is a hexagonal structure, type UCl₃, with the C_{3h} symmetry point of lanthanide. The LaCl₃ is an appealing material for investigations involving lanthanide ion spectroscopy due to its exceptional optical transparency, low phonon frequencies, low production costs, and low melting point temperature (Krämer *et al.*, 1998).

In this work, the alpha, proton, neutron, and gamma radiation interaction with LaCl₃:Yb crystal were investigated. The interaction parameters of photons, charged particles (alpha and proton) and neutron of the LaCl₃:Yb crystal were calculated by approaches using, FLUKA, WinXCom program, and SRIM & TRIM code.

Theoretical Background

Simulation setup

The mol percentage and density of the LaCl₃:Yb crystal are (99%)LaCl₃ and (1%)YbCl₃ and 3.64 g/cm³, respectively. The FLUKA Monte Carlo simulation programs (version 4.3.3) were used for investigating the photon's interaction with the LaCl₃:Yb crystal, as showed in Figure 1. The simulation details of narrow beam transmission were set following the previous study (Mutuwong *et al.*, 2018). In order to determine the total mass stopping power (TMSP) of the LaCl₃:Yb for alpha and proton particles within the energy range of 0.01 MeV to 10,000 MeV, the SRIM & TRIM programs were executed. Furthermore, SRIM & TRIM were utilized to examine the projected range, ion distribution, and ion ranges of the LaCl₃:Yb. The simulation was run with a total of 10,000 primary particles.

Photon interaction

The linear (μ) and mass attenuation coefficients (μ_m) of samples were calculated using the Lambert-Beer law (Chaiphaksa *et al.*, 2016):

$$\mu = \frac{1}{d} \ln \left(\frac{I_0}{I} \right), \quad (1)$$

$$\mu_m = \frac{1}{\rho d} \ln \left(\frac{I_0}{I} \right), \quad (2)$$

where the I_0 and I values correspond to the intensity of the photon when there is no sample and when there is a sample, respectively. The d and ρ indicate the thickness and density of the sample, respectively.

Theoretical values of μ_m for mixtures can be obtained by a weighted summation of the constituents in the NIST database by the XCOM program (Gerward *et al.*, 2004). This can be expressed mathematically as follows:

$$\mu_m = \sum w_i (\mu_m)_i \quad (3)$$

where the variable w_i represents the normalized weight fractions of i^{th} element. The $(\mu_m)_i$ is the mass attenuation coefficient of i^{th} element.

The mean free path (MFP) and half-value layer (HVL) can be mathematically expressed as follows:

$$\text{MFP} = \frac{1}{\mu}, \quad (4)$$

$$\text{HVL} = \frac{\ln(2)}{\mu} \quad (5)$$

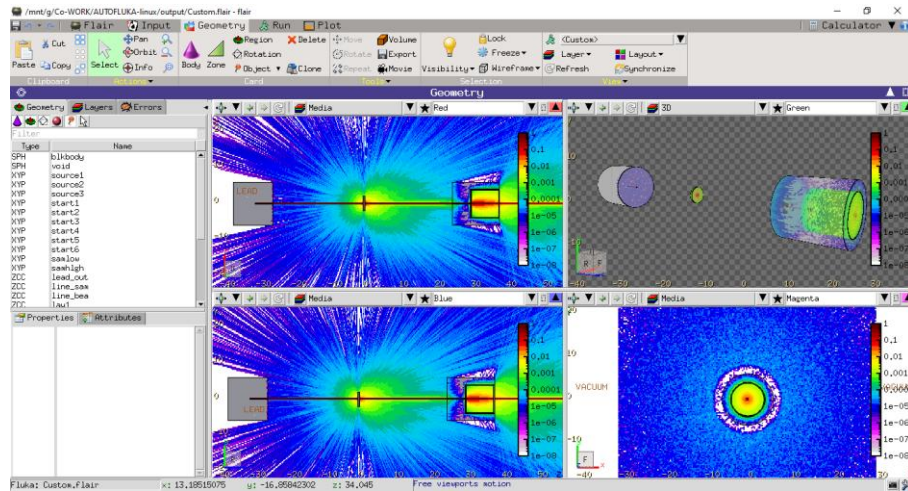


Figure 1. FLUKA simulation setup of narrow beam transmission

The total atomic cross-section ($\sigma_{t,a}$) is equal to the summation of partial cross-sections associated with photon interactions with atoms. The relationship between $\sigma_{t,a}$ and μ_m were expressed by the following equation (Hubbell, 2006):

$$\sigma_{t,a} = \frac{(\mu_m)_{\text{sample}}}{N_A \sum_i^n (w_i/A_i)} \quad (6)$$

where N_A is Avogadro's number. The A_i is the atomic weight of constituent elements of the mixture. The total electronic cross-section ($\sigma_{t,el}$) is the cross section by which photons interact with the electron, as expressed by the following equation (Cheewasukhanont *et al.*, 2020):

$$\sigma_{t,el} = \frac{1}{N_A} \sum_i^n \frac{f_i A_i}{z_i} (\mu_m)_i \quad (7)$$

where f_i denotes the fractional abundance of the element i with respect to the number of atoms ($\sum f_i = 1$) and z_i is the atomic number of i^{th} elements.

The effective atomic number (Z_{eff}) and the effective electron number or electron density (N_{eff}) of the composite material, as calculated using the following relation (Cheewasukhanont *et al.*, 2020):

$$Z_{\text{eff}} = \frac{\sigma_{t,a}}{\sigma_{t,el}}, \quad (8)$$

$$N_{\text{eff}} = \frac{\mu_m}{\sigma_{t,el}}. \quad (9)$$

Charged particle interaction

Charged particles experience energy dissipation as they traverse matter, as they impart their energy to excite and ionize the matter's atoms or molecules. The mass stopping power (TMSP) refers to the characteristics of materials that induce charged particles to lose energy proportionally to depth and density. This property is defined by the Bethe-Bloch formula (Braibant *et al.*, 2012).

$$\text{TMSP} = -\frac{1}{\rho} \frac{dE}{dx} = 2\pi N_A m_e r_e^2 c^2 \frac{Z}{A} \frac{z^2}{\beta^2} \left[\ln \left(\frac{2m_e \gamma^2 v^2 W_{\text{max}}}{I^2} \right) - 2\beta^2 - \delta - 2 \frac{C}{Z} \right] \quad (10)$$

where

$$\begin{aligned} r_e &= e^2/m_e c^2 \text{ classical electron radius} \\ 2\pi m_e r_e^2 c^2 &= 0.1535 \text{ MeV g}^{-1} \text{ cm}^2 \\ m_e &= \text{electron mass} = 9.110 \cdot 10^{-31} \text{ kg} \\ N_A &= \text{Avogadro's number} = 6.022 \cdot 10^{23} \text{ mol}^{-1} \end{aligned}$$

I = mean ionization(excitation) potential of target

ρ = material density

Z = atomic number of absorber medium

A = atomic weight of absorber medium

z_e = charge of the incident particle

$\beta = v/c$ of incident particle

$\gamma = 1/\sqrt{1 - \beta^2}$

δ = density effect correction (vital at high energy)

C = shell correction (already vital at low energy)

W_{max} = maximum kinetic energy imparted to an e^- in a single collision $\cong 2m_e c^2 (\beta\gamma)^2$, for $M \gg m_e$.

The TMSP is written, in general, as the sum of two terms (Tsoulfanidis and Landsberger, n.d.):

$$\text{TMSP} = \left(-\frac{1}{\rho} \frac{dE}{dx} \right)_{\text{total}} = \left(-\frac{1}{\rho} \frac{dE}{dx} \right)_{\text{elec.}} + \left(-\frac{1}{\rho} \frac{dE}{dx} \right)_{\text{nuclear}} \quad (11)$$

Where $\left(-\frac{1}{\rho} \frac{dE}{dx} \right)_{\text{elec.}}$ = electronic energy loss,

$\left(-\frac{1}{\rho} \frac{dE}{dx} \right)_{\text{nuclear}}$ = nuclear energy loss.

Neutron removal cross-section

The FNSR (Σ_R) values of the $\text{LaCl}_3:\text{Yb}$ crystal were expressed using the given equation (Chaiphaksa *et al.*, 2023):

$$\Sigma_R = \sum_i \rho_i (\Sigma_{R/\rho})_i \quad (12)$$

where $(\Sigma_{R/\rho})_i$ is the mass removal cross-section of i^{th} element and $\rho_i = w_i/\rho$ is partial density of i^{th} element.

Results and Discussion

Figure 2(a) and Figure 2(b) depict results of two-dimensional simulations of photon fluence at 0.662 MeV, both with and without a $\text{LaCl}_3:\text{Yb}$ crystal (thickness 0.2 cm), respectively. The results were performed by FLUKA program (Ahdida *et al.*, 2022) using the USRBIN scoring card with x-y-z mesh. The Compton scattering phenomena occurring when photons interact with $\text{LaCl}_3:\text{Yb}$ crystal was clearly demonstrated in Figure 2 (b). Moreover, the number of particles passing through the NaI(Tl) region was recorded by USRTRACK card in the absence and presence of the $\text{LaCl}_3:\text{Yb}$ crystal, respectively.

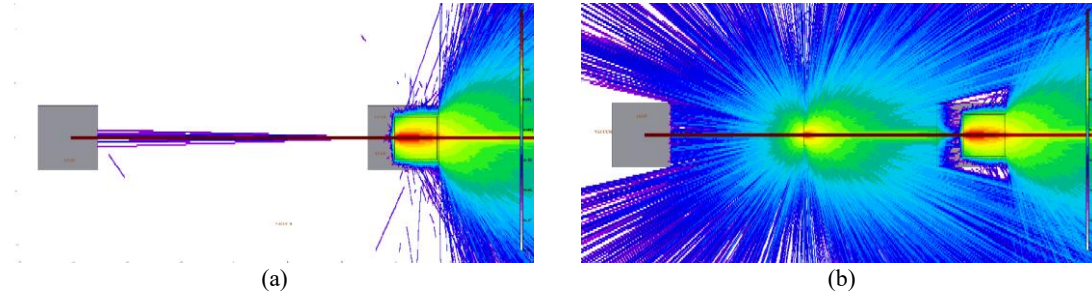


Figure 2. The photon fluence (photon/cm²) by FLUKA at 662 keV (a) without sample and (b) with sample

The variation in atomic cross-section as the energy of the incident photon changes can be ascribed to the three primary photon interaction processes that occur in distinct energy regions with $\text{LaCl}_3:\text{Yb}$. The total and partial atomic cross-sectional values of $\text{LaCl}_3:\text{Yb}$, as computed by FLUKA and XCOM, are depicted in Figure 3. The figure illustrates that the values of $\sigma_{t,a}$ for both calculations are identical. The photoelectric process is dominant at energy levels ($E < 0.2$ MeV), where $\sigma_{t,a}$ values are significantly high. At around 0.0392 MeV, $\sigma_{t,a}$ value dramatically rises due to the K-absorption edges of La (Alzahrani *et al.*, 2023). The total atomic cross-section decreases gradually in the ($0.2 \leq E \leq 6$ MeV) energy region because the Compton scattering atomic cross section is inversely proportional to the incident photon energy. At $E > 6$ MeV, the pair production becomes the dominant. The Z_{eff} and N_{eff} for $\text{LaCl}_3:\text{Yb}$ are depicted in Figure 4 and Figure 5, respectively. Clearly, the Z_{eff} are between 27.67 and 53.02 (electrons/atom), fluctuating dramatically with photon energy. The N_{eff} values range from 2.72 to 5.20 ($\times 10^{23}$ electrons/g) and vary considerably with photon energy.

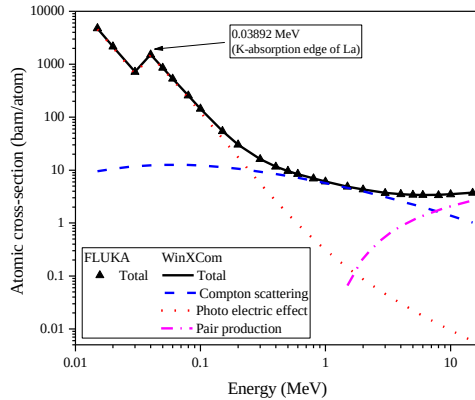


Figure 3. Atomic cross-section (barn/atom) of $\text{LaCl}_3:\text{Yb}$.

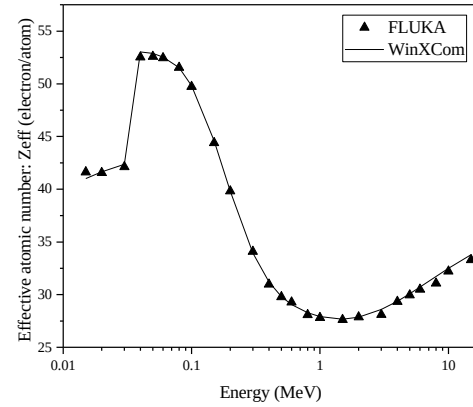


Figure 4. Z_{eff} (electron/atom) of $\text{LaCl}_3:\text{Yb}$.

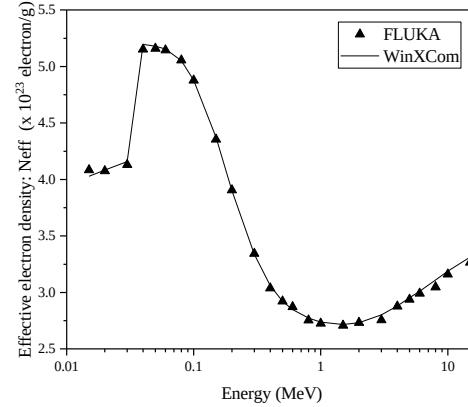


Figure 5. N_{eff} (electron/g) of $\text{LaCl}_3:\text{Yb}$.

The MFP and HVL of $\text{LaCl}_3:\text{Yb}$ are, respectively, illustrated in Figure 6 and Figure 7. The trends of MFP and HVL values exhibit an increase as energy increases.

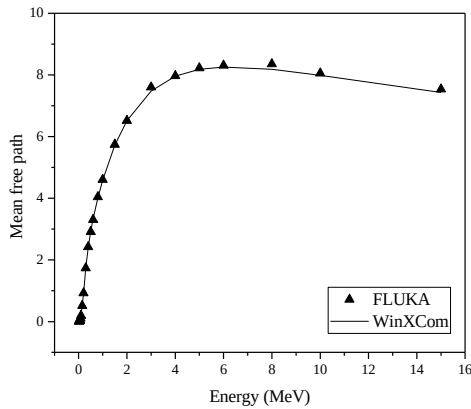


Figure 6. MFP (cm) of $\text{LaCl}_3\text{:Yb}$.

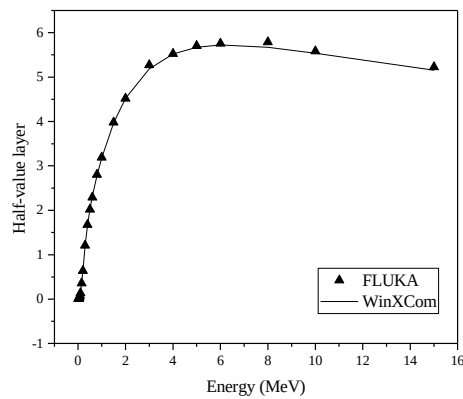


Figure 7. HVL (cm) of $\text{LaCl}_3\text{:Yb}$.

The SRIM & TRIM programs (Ziegler *et al.*, 2010) are utilized to investigate the TMSP, projected range (PR), ion distribution, and ion ranges of the $\text{LaCl}_3\text{:Yb}$ scintillator with respect to alpha and proton particles. The TMSP of $\text{LaCl}_3\text{:Yb}$ is illustrated in Figure 8. According to the findings, electronic energy loss has a greater effect on TMSP than nuclear energy loss. The maximum values of TMSP are approximately $353.985 \text{ (MeV cm}^2\text{/g)}$ at a proton energy of 0.09 MeV and $981.045 \text{ (MeV cm}^2\text{/g)}$ at an alpha energy of 0.6 MeV , respectively. The energy loss, also known as the total mass-stopping power curve, is energy-dependent. As a result, incoming high-energy particles incur a minimal energy loss denoted as dE/dx . However, the energy loss reaches its maximal value when the particles have decelerated to energies that correspond to the peak of the energy loss curve (El-Ghossain, 2017). The TMSP indicates the potentiality of a material to reduce the kinetic energy of particles traveling toward it by ionizing the molecules.

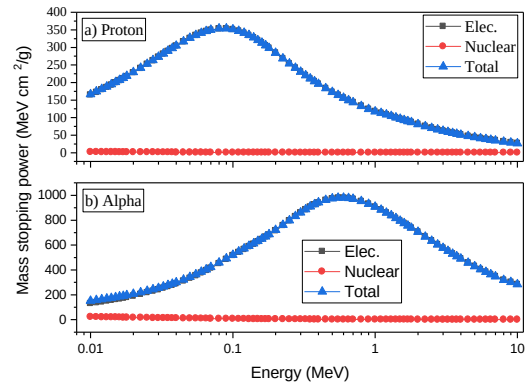


Figure 8. TMSP ($\text{MeV cm}^2\text{/g}$) of $\text{LaCl}_3\text{:Yb}$ for a) proton and b) alpha

The projected range (PR) refers to average value of the depth to which a charged particle will penetrate in the course of slowing down to rest. Figure 9 illustrates the correlation between the PR of $\text{LaCl}_3\text{:Yb}$ and their kinetic energy. The results indicate that the projected range of alpha and proton particles penetrating the $\text{LaCl}_3\text{:Yb}$ increases with increasing energy. Furthermore, it can be observed that proton particles exhibit a greater projected range in comparison to alpha particles of the same energy. This is because proton particles have more penetration power than alpha particles.

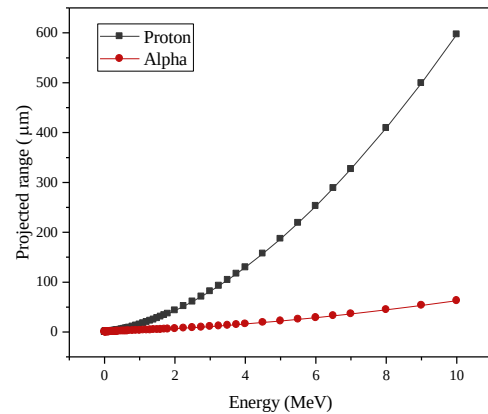


Figure 9. Projected range of $\text{LaCl}_3\text{:Yb}$ as a function of energy

Figure 10 and Figure 11 depict, respectively, the outcomes of the two-dimensional simulation of the ion distribution generated by proton particle and alpha particle interactions with $\text{LaCl}_3:\text{Yb}$ at energies of 0.01 MeV and 0.05 MeV. The results indicate that the maximal probability distributions of ion ranges are as follows: $0.1337 \mu\text{m}$ for a proton

energy of 0.01 MeV and $0.4649 \mu\text{m}$ for a proton energy of 0.05 MeV. The maximum probability distributions of alpha's ion ranges are $0.1028 \mu\text{m}$ for 0.01 MeV proton energy and $0.3835 \mu\text{m}$ for 0.05 MeV alpha energy. The FNSR value of the $\text{LaCl}_3:\text{Yb}$ crystal is 0.066 cm^{-1} .

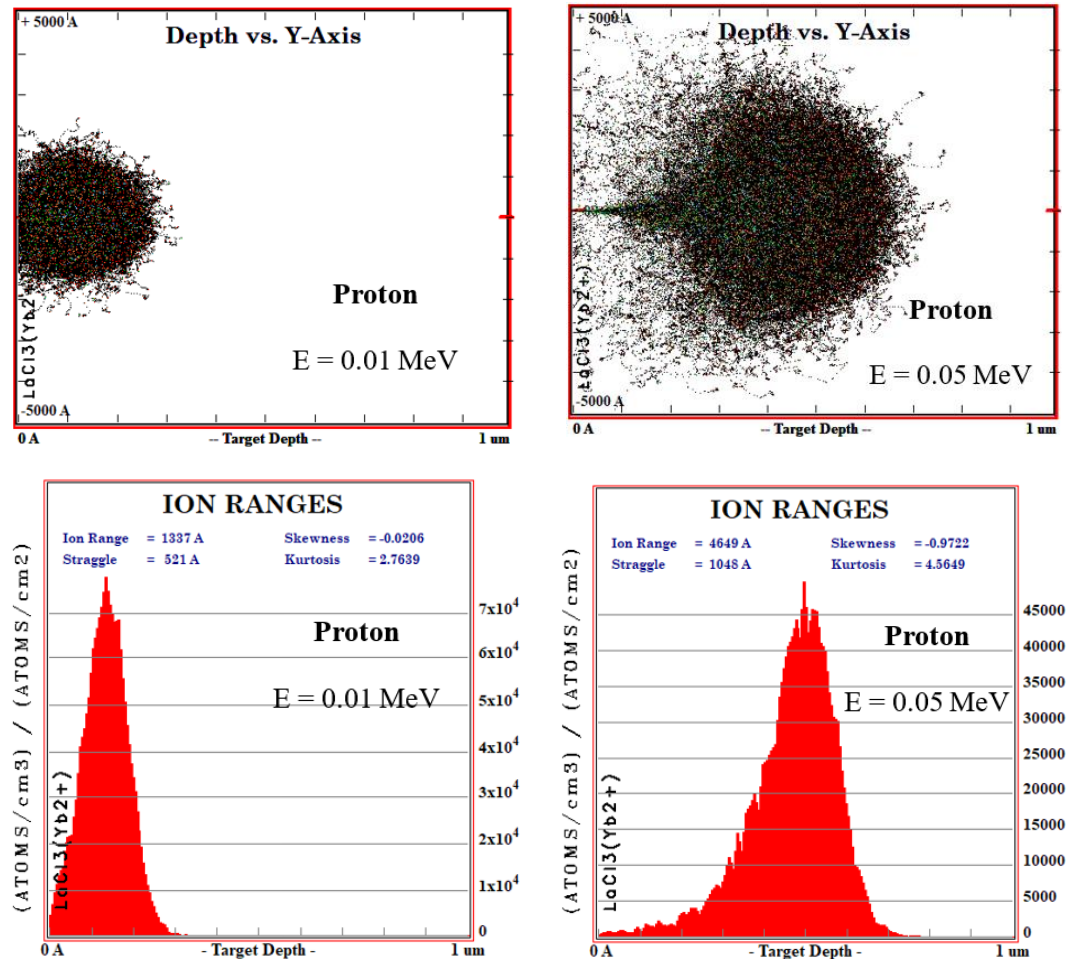


Figure 10. The 2D Monte Carlo simulation of the 10,000 proton particles interact with the $\text{LaCl}_3:\text{Yb}$ at energies 0.01 MeV and 0.05 MeV, and the probability distributions of ion ranges at 0.01 MeV and 0.05 MeV.

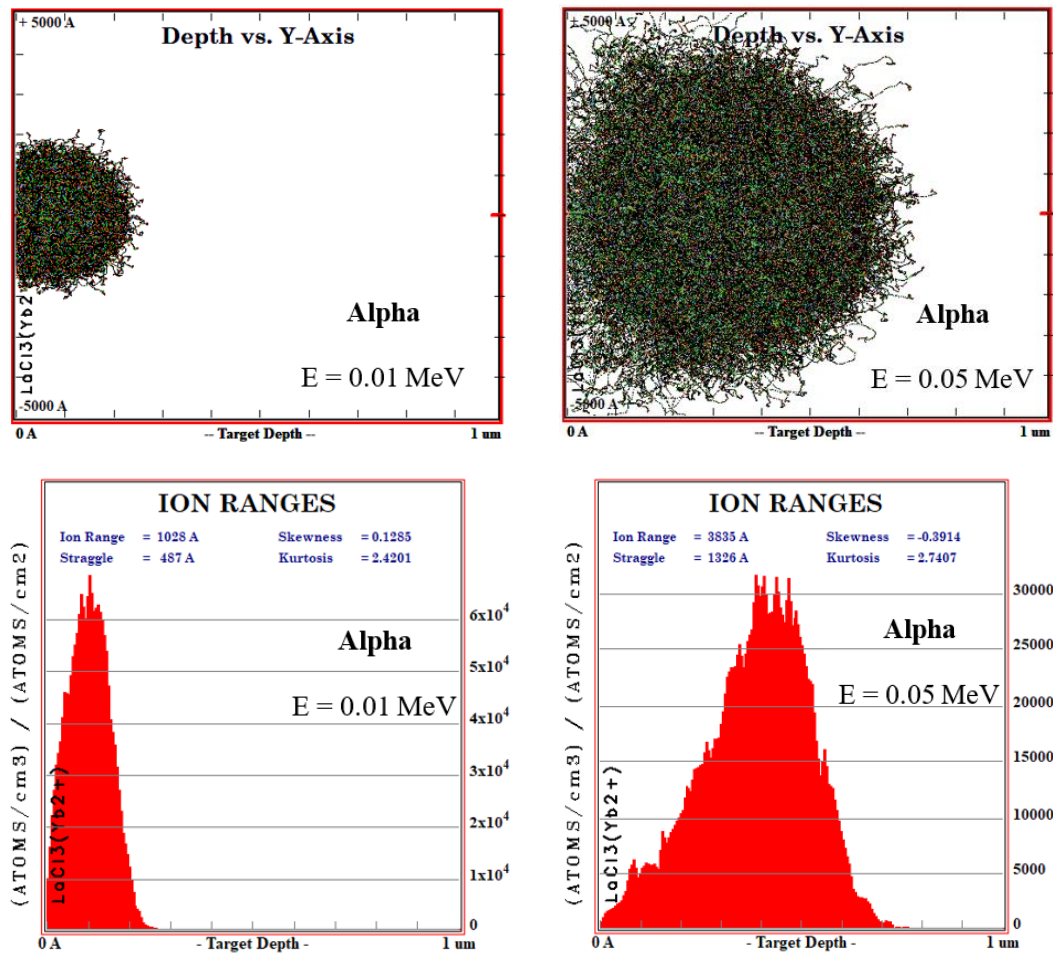


Figure 11. The 2D Monte Carlo simulation of the 10,000 alpha particles interact with the LaCl₃:Yb at energies 0.01 MeV and 0.05 MeV, and the probability distributions of ion ranges at 0.01 MeV and 0.05 MeV.

Conclusions

The interaction of alpha, proton, neutron, and gamma radiation with the LaCl₃:Yb crystal was investigated by TRIM & SRIM code, the WinXCom program, and Monte Carlo simulation. In this work, the total atomic cross-section ($\sigma_{t,a}$), effective atomic number (Z_{eff}), effective electron density (N_{eff}), half-value layer (HVL), mean free path (MFP), total mass stopping power (TMSP), and projected range (PR) are computed. The results of the simulation indicate that the photon interaction parameters calculated by the programs FLUKA and WinXCom are highly similar. The Z_{eff} are between 27.67 and 53.02 (electrons/atom). According to the results, the LaCl₃:Yb crystal can be utilized for a variety of photon, charged particle, and neutron detection applications.

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