**Jurnal Ilmu Fisika**
Vol. 16, No. 2, September 2024, pp. 166–176
ISSN: 1979-4657 (Print); 2614-7386 (Online)
https://doi.org/10.25077/jif.16.2.166-176.2024

Jurnal Ilmu Fisika
Open Access

# Simulation of the Effect of $Dy^{3+}$ Dopant on the Mass Energy Absorption Coefficient and Relative Energy Response of TLD Made from Lithium Magnesium Borate Using MCNP

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**Article Info**

***Article History:***

Received April 26, 2024
Revised July 31, 2024
Accepted August 05, 2024
Published online August 15, 2024

***Keywords:***

*MCNP*
*TLD*
*LMBDy$^{3+}$*
*mass energy absorption coefficient*
*relative energy response*

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**ABSTRACT**

Thermoluminescence dosimeter (TLD) is widely used as a personal and medical dosimeter. Several TLD materials show the characteristics of mass energy absorption coefficient and energy response relative to ICRU (International Commission on Radiation Units and Measurements) issue material as an equivalent material for human body soft tissue. This research aims to analyze the effect of Dy3+ dopant on the mass-energy absorption coefficient and relative energy response of Lithium Magnesium Borate (LMB) materials. The simulation was carried out using Monte Carlo N-Particle (MCNP) software. Calculations based on simulation and theoretical results will be compared statistically using paired t-tests. The study showed that adding a Dy3+ dopant to TLD material made of Lithium Magnesium Borate (LMB) only affected the mass-energy absorption coefficient and relative energy response for low radiation energy. Adding Dy3+ dopant increased the mass energy absorption coefficient and relative energy response in a reasonably small value. Based on these results, LMBDy3+ produces a better mass-energy absorption coefficient value for TLD materials. The results of the statistical tests show a significant difference in the mass energy absorption coefficient value. At the same time, there is no significant difference between the simulation results and theoretical calculations for the relative energy response.

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## 1. INTRODUCTION

Ionizing radiation, such as γ-rays and X-rays, has been widely developed for radiotherapy because of its advantages. The advantage of ionizing radiation is its unique characteristic of penetrating power towards materials. With this ability, it can be used in the medical world to kill cells in the human body without invasive treatment (Gordon, 2023). Radiotherapy itself is a form of treating cancer patients using radiation. The radiation sources used can be X-rays, $\gamma$-rays, and neutron particles. Meanwhile, the energy range that is widely used ranges from 0.02 MeV to 20 MeV (Redd, 2003; Terasawa et al., 2009).

Ionizing radiation in radiotherapy can damage healthy body tissue, so it is important to anticipate this effect and ensure that the treatment is accurately targeted. In addition to setting the patient in an invariable radiation scope, measuring the dose released from the radiation source is essential in planning radiotherapy. Therefore, dosimeters are crucial in ensuring the quality of the patient's dose and

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whether the radiation dose produced by the radiation source is accurate and appropriate. A thermoluminescence dosimeter (TLD) is one of the dosimeters that can be used to measure radiation dose (Maruyama et al., 2020).

TLD is a dosimeter used in scientific fields such as personal, clinical, and environmental research related to radiation exposure and applied fields such as radiation protection (Bakhsh et al., 2018; Yeni et al., 2019). This TLD is included in the passive dosimeter category, which does not require energy in radiation, so with this advantage, the dosimeter can be used for measurement purposes at a more affordable cost (Petrovi et al., 2021). For various dosimetric applications, a single robust, tissue-equivalent, extremely sensitive thermoluminescence dosimeter with exceptional signal stability is always preferred (Bakhsh et al., 2022). Based on the European Radiation Dosimetry (EURADOS) report, more than 80% of European radiation exposure levels measured by related service providers in 2016 used thermoluminescence dosimeters (Harrison et al., 2021). Meanwhile, the thermoluminescence (TL) material that is widely used is lithium fluoride (LiF) with various dopants (Duch et al., 2021).

The use of TLD as a tool for monitoring exposure to ionizing radiation in the medical realm makes it essential to study the interaction of photons with TL materials because TLD is considered a tissue equivalent. The dosimeter, which is positioned as a material equivalent to the TL tissue used, has a mass energy absorption coefficient ($\mu_{en}/\rho$) and energy response equivalent to human tissue in the same situation (Chand et al., 2021; Petrovi et al., 2021; Souza et al., 2019). The mass energy absorption coefficient is a coefficient that can be used to determine the amount of photon energy used to produce chemical and biological effects associated with exposure to ionizing radiation. Therefore, this coefficient helps estimate medical and health physics absorption levels. Meanwhile, the energy response helps determine energy correction methods in TL materials (Souza et al., 2019).

TLD development from the aspect of its constituent materials continues to be carried out to achieve the ideality of the TLD itself as a radiation dosimeter. TLD is an ideal dosimeter if it has a linear dose response for all energy ranges, high sensitivity, network equality, reproducibility, and stability of the TL signal (Yukihara & McKeever, 2011). Lithium fluoride (LiF) and carbon-doped aluminum oxide ($Al_2O_3$:C) have been commercially used as TLD materials. Even though it has several advantages, this material has a relatively high mass energy absorption coefficient value and a relative energy response that shows an over-response value when compared with equivalent material for human body soft tissue (ICRU tissue). Development of the $MgB_4O_7$ material by Souza et al. (2019) also produced higher mass energy absorption coefficient and relative energy response values compared to the ICRU (International Commission on Radiation Units and Measurements) tissue (Souza et al., 2019). Therefore, it is necessary to develop TLD materials to achieve mass energy absorption coefficients and relative energy responses equivalent to ICRU tissue.

Lithium borate (LB) glass is one of the various TL materials utilized for dosimetry; it has been extensively researched due to its promising properties (Bakhsh et al., 2018). Such LB glass's characteristics are high sensitivity, close to tissue equality, and stress-free manufacturing. However, this material has disadvantages, namely low TL peak intensity and short luminescence, so some scientists have engineered the material by adding magnesium metal. This engineering produces a new material, lithium magnesium borate (LMB), with improved performance compared to LB material, such as hardness, TL signal stability, and good linearity over a wide dose range (Ahamad et al., 2021).

However, on the other hand, LMB has several detrimental aspects when viewed from a radiation dosimetry perspective, such as fading caused by light, low peak TL intensity, and short-term luminescence (Ahamad et al., 2021; Anishia et al., 2011). The solution that can be taken to overcome this problem is to add rare earth elements to the LMB so that TLD performance increases because rare earth metal ions can activate the TL material as a luminescent center (Kaur et al., 2019). Dysprosium(III) ion ($Dy^{3+}$) can be used as a dopant because this element has a linear dose-response, increases TL sensitivity, strengthens the TL intensity peak, and increases the luminescence period (Hashim et al., 2019). However, TLDs made from LMB and LMB$Dy^{3+}$ need to be evaluated for their mass energy absorption coefficient characteristics and relative energy response when used as personal and medical dosimeters, and research still needs to be done.

From this perspective, TLD simulations using lithium magnesium borate (LMB) doped with $Dy^{3+}$ (LMB: $Dy^{3+}$) must be carried out to determine the mass energy absorption coefficient and relative energy response. The software used in this study to conduct simulations is Monte Carlo N-Particle (MCNP). MCNP is software that uses Monte Carlo as the basis of its computing method. The Monte Carlo is a stochastic method that utilizes random sampling techniques to solve complex multidimensional integral equation problems. One application of MCNP problem-solving is medical physics problems, including dosimetry (Fielding, 2023).

## 2. METHOD

### 2.1 The equation for the mass-energy absorption coefficient and RER

The value of the mass-energy absorption coefficient ($\mu_{en}/\rho$) and the relative energy response (RER) in the MCNP simulation were calculated using Equations (1) and (2). Meanwhile, for the theoretical calculation, the value of the mass-energy absorption coefficient and the relative energy response (RER) were calculated using Equations (4) and (5). The $\omega_i$ and $(\mu_{en}/\rho)_i$ respectively, are the weight fraction and mass energy absorption coefficient of each element present in a compound. The relative difference (RD) between the simulation and theoretical studies results was calculated using Equation (3). The tally code *F6* represents the energy deposition per particle emitted by the source and **F4* represents the fluence energy.

$$\left(\frac{\mu_{en}}{\rho}\right)_{Simulation} = \frac{F6\left(\frac{MeV/g}{particle}\right)}{{}^{*}F4\left(\frac{MeV/g}{particle}\right)} \quad (1)$$

$$RER = \frac{\left(\frac{\mu_{en}}{\rho}\right)_{TLD,Simulation}}{\left(\frac{\mu_{en}}{\rho}\right)_{Reference,Simulation}} \quad (2)$$

$$RD(\%) = \left|\frac{\left(\frac{\mu_{en}}{\rho}\right)_{Simulation} - \left(\frac{\mu_{en}}{\rho}\right)_{Theoretical}}{\left(\frac{\mu_{en}}{\rho}\right)_{Theoretical}}\right| \quad (3)$$

$$\left(\frac{\mu_{en}}{\rho}\right)_{Theoretical} = \sum_i^n \omega_i \left(\frac{\mu_{en}}{\rho}\right)_i \quad (4)$$

$$RER = \frac{\left(\frac{\mu_{en}}{\rho}\right)_{TLD,Theoretical}}{\left(\frac{\mu_{en}}{\rho}\right)_{Reference,Theoretical}} \quad (5)$$

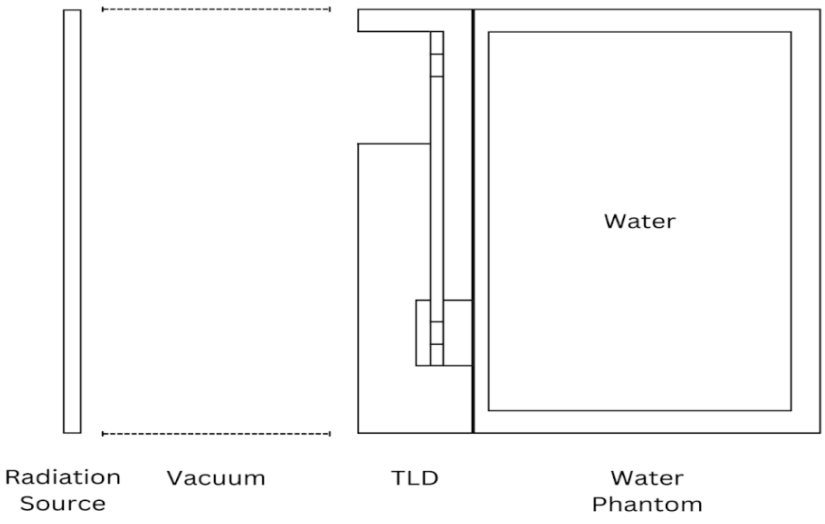


**Figure 1** TLD simulation design using MCNP.

### 2.2 Simulation

MCNP is software based on the Monte Carlo (MC) computing method that can simulate the interaction of radiation with matter. MCNP's field of application includes calculating fundamental dosimetry quantities to simulate radiotherapy treatment planning (Andreo, 2018). Several supporting applications are needed to use MCNP6 software for particle simulation, such as Notepad++, Visual Editor (Vised), and Total Commander. Notepad++ functions for modifying program code, Vised functions for displaying program code geometry, and Total Commander functions for data sampling.

In this simulation, the TLD is placed in a thin container made of plastic material with a depth of 1 mm, as shown in Figure 1. TLD has dimensions of 3.2 mm x 3.2 mm x 1.0 mm with a density of 2.20 g/cm$^3$; an illustration of TLD chip front and rear view in simulation design can be seen in Figure 2. A radiation source from a distance of 100 cm irradiates the TLD, resulting in an area of 10 cm x 10 cm of light radiation that exposes the TLD. *Polyethylene* is the material used to wrap TLDs. The simulation configuration is used consistently with changes in the materials making up the dosimeter, as presented in Table 1.

**Table 1** The weight fraction of each element present in the material used in the simulation (Bos, 2001; Hashim et al., 2019).

| Element | Weight Fraction (%) | | | |
|---|---|---|---|---|
| | **LiF:Mg,Ti ($Z_{eff}$ = 8.27)** | **LMB ($Z_{eff}$ = 7.34)** | **LMB$Dy^{3+}_{0.1\%}$ ($Z_{eff}$ = 8.13)** | **ICRU Tissue ($Z_{eff}$ = 7.35)** |
| Li | 0.2672 | 0.1667 | 0.1667 | - |
| F | 0.73259 | - | - | - |
| Mg | 0.0002 | 0.0260 | 0.0110 | - |
| Ti | 0.00001 | - | - | - |
| O | - | 0.6118 | 0.5703 | 0.762 |
| H | - | - | - | 0.101 |
| C | - | - | - | 0.111 |
| N | - | - | - | 0.026 |
| Dy | - | - | 0.0008 | - |

The radiation source emits light isotropically with a simulated number of photon particles of 50 million particles. The photon energy that will be used starts from 0.02 MeV to 20 MeV with 25 variations. The variations in the energy range refer to research by Hubbell & Seltzer (2004). The energy that will be measured in this simulation is the energy deposited on the material represented by Tally F6 (MeV/g/particle) and the energy flux in the cell defined by Tally *F4 (MeV/cm$^2$/particle). TLD with LiF:Mg,Ti material is used as a comparison because it is the standard material used for TLD.

## 3. RESULTS AND DISCUSSION

### 3.1 Mass Energy Absorption Coefficient

The calculation of the value of the mass-energy absorption coefficient through simulation is obtained from the process of running the program code using Total Commander, which produces Tally data F4 and F6. Meanwhile, the theoretical mass-energy absorption coefficient data is obtained by calculating the mass-energy absorption coefficient of each component of the TLD material with the help of Spreadsheet. The comparison of the results of calculating the mass-energy absorption coefficient by simulation and theoretically for LiF:Mg,Ti; LMB; LMB$Dy^{3+}$, and ICRU tissue is displayed graphically in Figure 3. The effect of adding $Dy^{3+}$ dopant to LMB material on the mass-energy absorption coefficient value is presented in Figure 4.

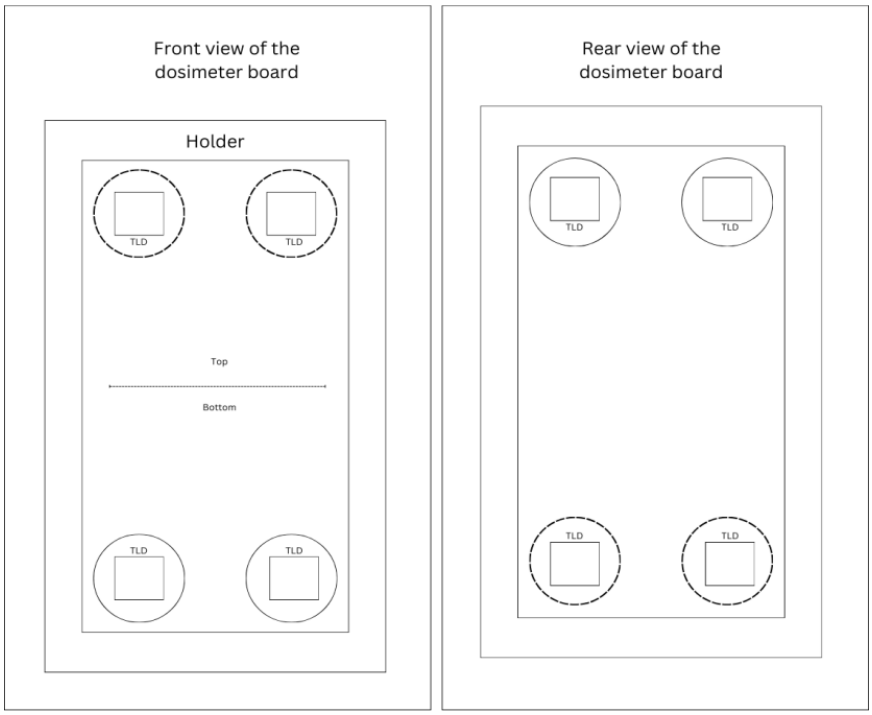


**Figure 2** Illustrates the TLD chip's front and rear view in the MCNP simulation.

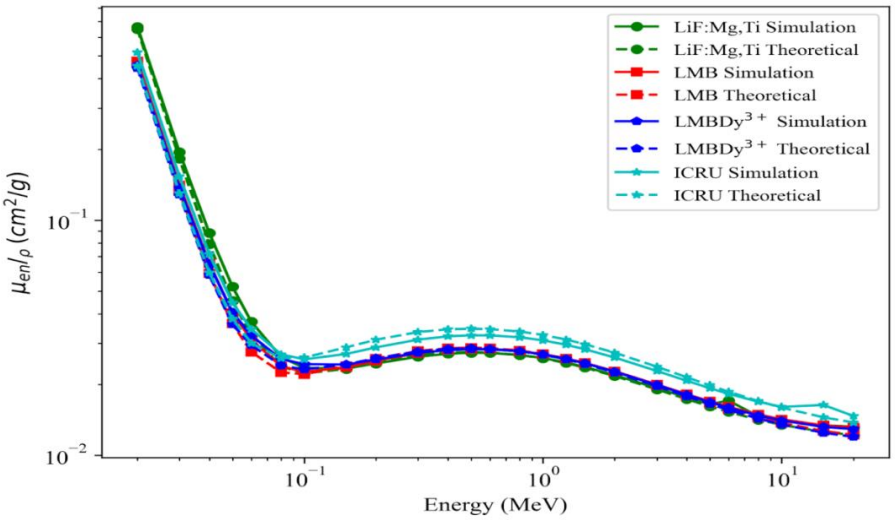


**Figure 3** Mass energy absorption coefficients

The photon energy range below 0.08 MeV shows a high mass-energy coefficient value for all TLD materials (Figure 3). In this energy range, the photoelectric effect dominates compared to the other impacts. This photoelectric effect occurs due to the interaction of photons with electrons in atomic orbits, allowing energy to be absorbed. The cross-section of the atomic interaction in this effect is proportional to 1/E3, which shows that photoelectric absorption decreases as the exposed energy increases (Attix, 2004; Souza et al., 2019).

In addition, the LiF:Mg,Ti material has a higher mass-energy absorption coefficient value than the other materials. This high value is due to the dependence of the mass-energy absorption coefficient on the effective atomic number ($Z_{eff}$). The influence of $Z_{eff}$ on the mass energy absorption coefficient is proportional to $Z_{eff}\ m$ with a value of $m$ = 4 for low photon energy and $m$ = 5 for high photon energy ($hv > 10\ MeV$). $Z_{eff}$ of LiF:Mg,Ti is worth 8.27, as presented in Table 1.

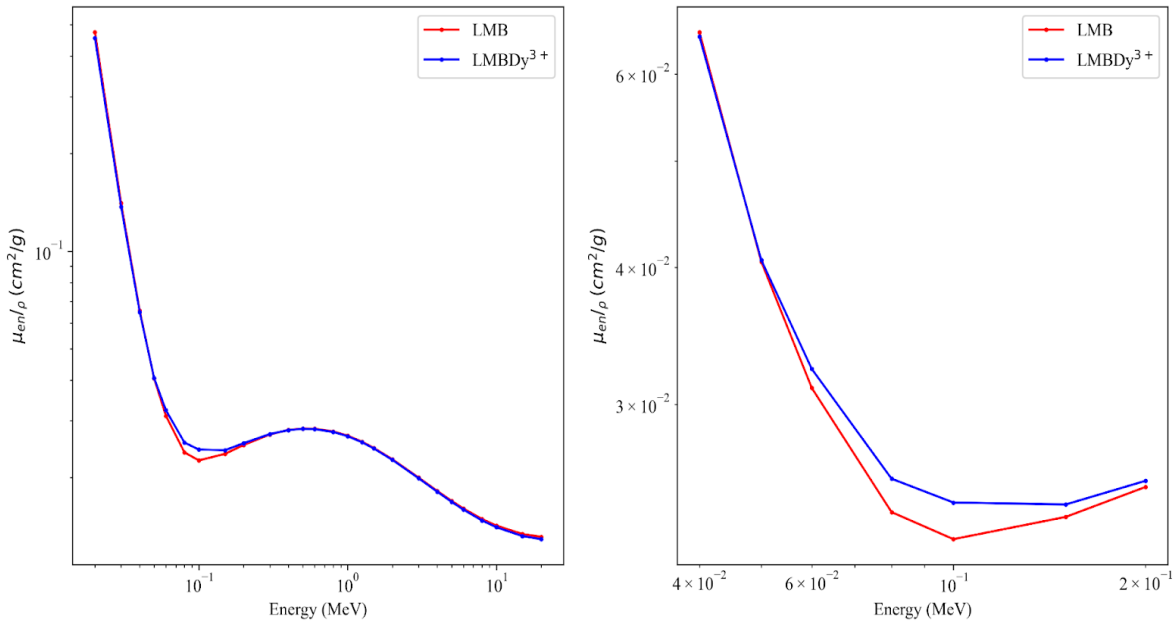


**Figure 4** Mass energy absorption coefficient LMB vs $LMBDy^{3+}$ for (a) all energy ranges and (b) the energy range 0.04 to 0.2 MeV

The results of this study, following research conducted by Souza et al. (2019), show a trend in which the mass energy absorption coefficient decreases as the energy of the exposed photons increases. However, the results of this study also show that there is a discrepancy in the results of the $LMBDy^{3+}$ mass-energy absorption coefficient with its correlation due to the $Z_{eff}$ value produced in the research of (Hashim et al., 2019) with a $Z_{eff}$ $LMBDy^{3+}$ value of 8.13. Based on this value of $Z_{eff}$ $LMBDy^{3+}$, the resulting mass-energy absorption coefficient should be close to the mass-energy absorption coefficient of LiF:Mg,Ti with a value of $Z_{eff}$ LiF:Mg,Ti of 8.27. This requires further investigation regarding $Z_{eff}$ $LMBDy^{3+}$ by carrying out theoretical calculations to obtain the value of $Z_{eff}$ $LMBDy^{3+}$.

Adding $Dy^{3+}$ dopant to the LMB matrix affects the mass-energy absorption coefficient in the energy range of 0.06 MeV to 2.00 MeV, as shown in Figure 4. The mass energy absorption coefficient increases with the addition of $Dy^{3+}$ dopant to LMB, ranging from 0.01 $cm^2/g$ to 0.02 $cm^2/g$. These results indicate that adding a $Dy^{3+}$ dopant to the LMB matrix affects the dependence of the mass-energy absorption coefficient on radiation energy. Charubala et al. (2019) conducted similar research examining TLD from the lithium magnesium borate doped with terbium (LMB:Tb) material for dosimetry eye lenses. This study evaluated the energy response with Monte Carlo based on the Fluka Code. The type of material strongly influences the energy response from the TLD. These results follow the research of Efenji et al. (2024), which states that the TLD materials' structural characteristics are essential to their dosimetric performance, including chemical composition, crystal structure, grain size, and annealing temperature.

### 3.2 Relative Energy Response (RER)

The Relative Energy Response (RER) value for each TLD material has been calculated by simulation and theory for the energy range of 0.02 MeV to 20.00 MeV. The calculation results are presented graphically in Figure 5. The RER value is the ratio of the mass-energy absorption coefficient of the TLD material to the ICRU tissue. The RER value of LMB and LMB3+ in the low energy range (below 0.10 MeV) approaches 1. The RER value decreases for higher energy ranges. The ideal RER value is 1, which states that the mass-energy absorption coefficient value of the TLD material studied is the same as the ICRU tissue value.

The RER obtained on the LiF:Mg,Ti material shows a higher relative energy response compared to LMB and $LMBDy^{3+}$ (Figure 5). This RER value is related to the dependence of the mass-energy

absorption coefficient on $Z_{eff}$ so that LiF:Mg,Ti, which causes a relatively higher energy response as well Yukihara & McKeever (2011). LMB and $LMBDy^{3+}$ display a relative energy response value smaller than the ideal value because the $Z_{eff}$value is smaller than ICRU tissue. There are differences in the values of simulation results and theoretical calculations, which can be due to differences in irradiation schemes such as the shape and thickness of the TLD, the irradiation distance used, the shape of the radiation source, and the irradiation model.

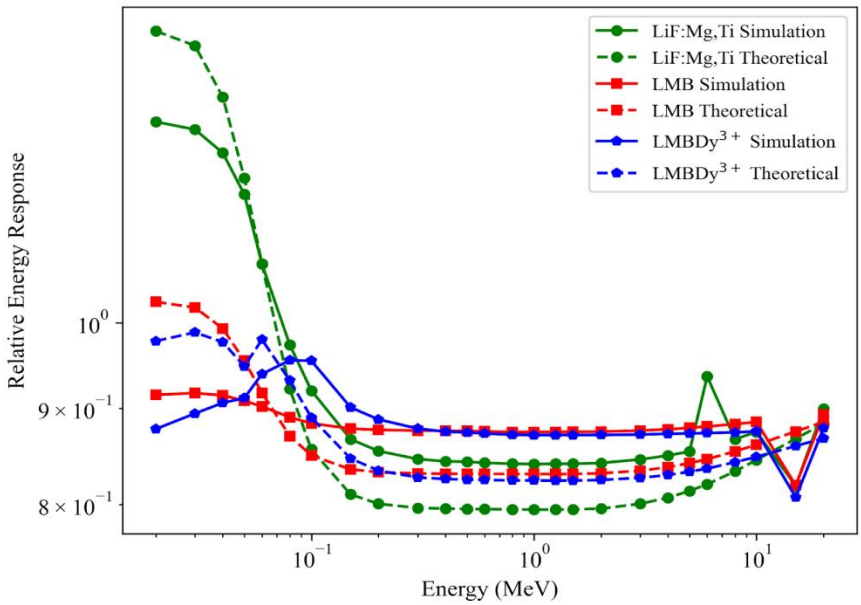


**Figure 5** Simulated and theoretical relative energy response of materials.

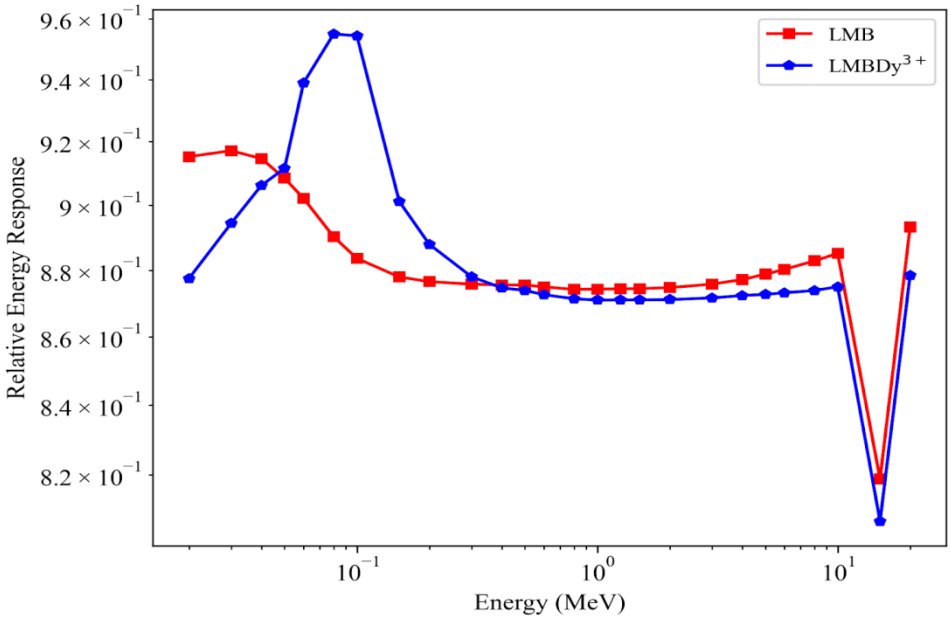


**Figure 6** Relative energy response of LMB vs $LMBDy^{3+}$.

The effect of adding a $Dy^{3+}$ dopant to LMB on the RER value is shown in Figure 6. The RER of the $LMBDy^{3+}$ material shows values close to ideal conditions in the energy range of 0.06 and 0.08 MeV, with RER values reaching 0.96. Meanwhile, in the energy range below 0.06 MeV and above 0.08 MeV, the RER value is below the ideal value (under-response).

The influence of the $Dy^{3+}$ dopant in the LMB matrix on the RER, as seen in Figure 6, is almost in all energy ranges except at the energy of 0.4 MeV, which shows relatively small changes in the energy response value. $Dy^{3+}$ dopant with a concentration of 0.1% reduces the relative energy response value in the energy range below 0.05 MeV and above 0.4 MeV compared to LMB without $Dy^{3+}$ dopant. Meanwhile, in the energy range of 0.05 to 0.3 MeV, the increase occurred after adding the $Dy^{3+}$ dopant.

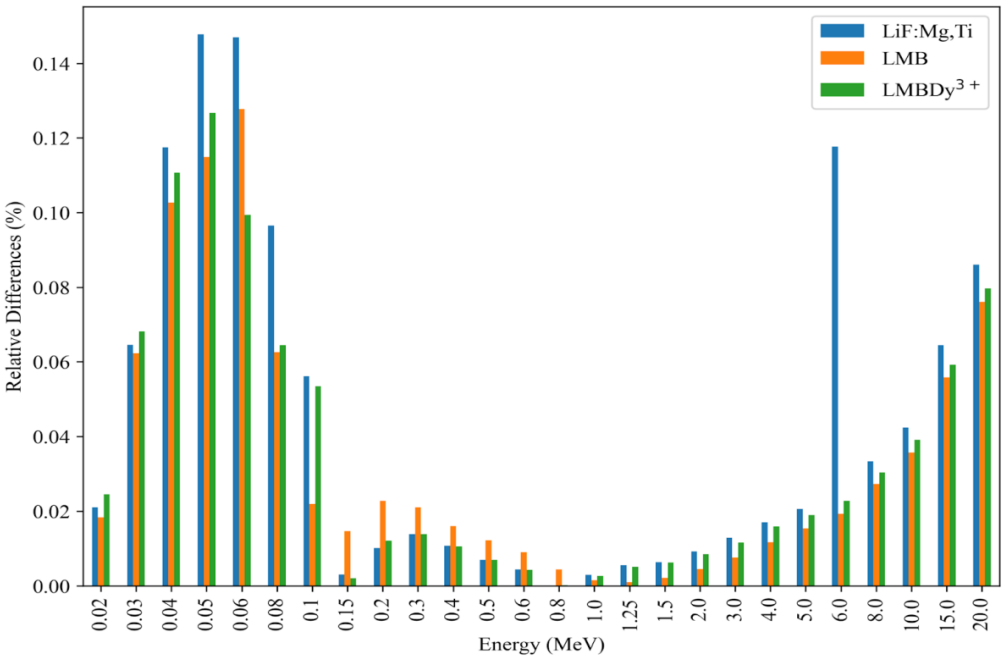


**Figure 7** Relative difference (%) of the mass-energy absorption coefficient.

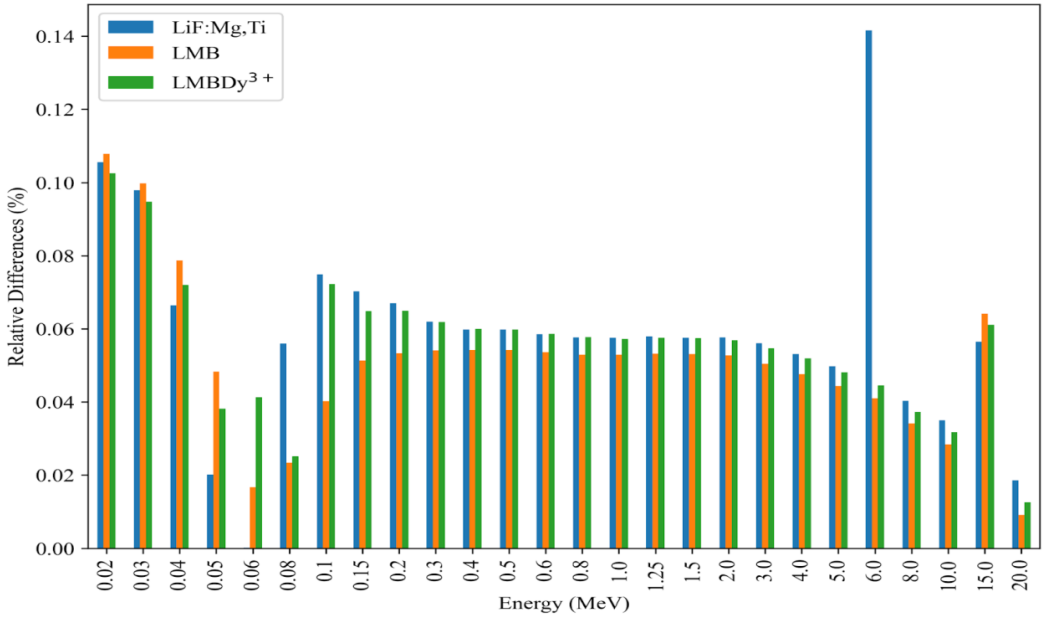


**Figure 8** Relative difference (%) of the relative energy response.

### 3.3 Statistical Analysis

This study calculated the mass-energy absorption coefficient and relative energy response values by simulation with MCNP software and confirmed them with theoretical calculations. The

difference in the results of the two calculation methods is expressed in the Relative Difference (%) value. The relative difference in the mass-energy absorption coefficient and relative energy response values are presented in Figures 7 and Figure 8, respectively. The highest relative difference (%) of the mass-energy absorption coefficient for the LiF:Mg,Ti material is 0.15%, LMB is 0.13%, and $LMBDy^{3+}$ is 0.13%. Meanwhile, the highest relative difference (%) of the relative energy response for the LiF:Mg, Ti material is 0.14%, LMB is 0.11%, and $LMBDy^{3+}$ is 0.10%. The high relative difference value at 6 MeV energy in calculating mass energy absorption coefficient and relative energy response is caused by an error in the simulation process. This anomaly can be disregarded because it only manifests at one energy within a wide range of energies. Further testing was carried out using statistical tests to see whether there were significant differences between the two methods used.

The paired *t*-test was conducted to determine whether there is a significant difference between the simulation results and theoretical calculations of mass energy absorption coefficients and relative energy responses. The significance level used in this statistical test is 95%. The statistical test results are expressed by the *p-value*, as presented in Table 2. The *p-value* < 0.05 indicates a significant difference between the simulation results and theoretical calculations of the two parameters: mass energy absorption coefficients and relative energy responses.

The mass-energy absorption coefficient t-test resulting from simulations and theoretical calculations for the LiF:Mg,Ti material has a p-value of 0.025, LMB has a *p-value* of 0.029, and $LMBDy^{3+}$ has a *p-value* of 0.021 (Table 2). These three TLD materials show a *p-value* smaller than the significance level (*p-value* < 0.05), illustrating a significant difference between the simulation and theoretical calculation results. The significant differences between simulations and theoretical calculations are possible due to the different parameters used to determine the mass-energy absorption coefficient, such as using different irradiation scenarios. This difference is because, in this study, several simplifications were made in the TLD radiation simulation process, such as TLD dimensions, radiation distance, and radiation collimation.

**Table 2** The *t*-test results for mass energy absorption coefficient.

| TLD Material | *p-value* | |
|---|---|---|
| | **mass energy absorption coefficient** | **relative energy response** |
| LiF:Mg,Ti | 0.025 | 0.111 |
| LMB | 0.029 | 0.175 |
| $LMBDy^{3+}{}_{0.1\%}$ | 0.021 | 0.073 |

The results of the *t*-test statistical test of the relative energy response based on the simulation results and theoretical calculations for LiF:Mg, Ti materials have a *p-value* of 0.111, LMB has a *p-value* of 0.175, and $LMBDy^{3+}$ has a *p-value* of 0.073. These three TLD materials show a *p-value* more significant than the significance level (*p-value* > 0.05), illustrating no considerable difference between the simulation and theoretical calculation results. This result means that the two methods used to calculate the relative energy response produce the same values.

## 4. CONCLUSION

The study of the effect of adding $Dy^{3+}$ dopant on the value of mass energy coefficient and relative energy response has been successfully carried out by simulation using the MCNP program. The impact of adding $Dy^{3+}$ dopant to LMB on the mass-energy absorption coefficient is seen in the photon energy range of 0.06 MeV to 2.00 MeV. The mass-energy absorption coefficient increased because adding a $Dy^{3+}$ dopant affected the increase in the effective atomic number ($Z_{eff}$) value of LMB material. The addition of $Dy^{3+}$ dopant also affected the relative energy response in the energy range of 0.06 MeV and 0.08 MeV, where the value was close to 1. From this study's results, adding a $Dy^{3+}$ dopant only affects the use of low photon energy for TLD irradiation.

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