Nanoscale calculation of the relative efficiency of $^7$LiF:Mg,Ti (MTS-7) and $^7$LiF:Mg,Cu,P (MCP-7) thermoluminescent detectors for measuring electrons and positrons

Alessio Parisi, Lara Struelens and Filip Vanhavere
Belgian Nuclear Research Centre SCK CEN, Boeretang 200, Mol, Belgium
E-mail: alessio.parisi@sckcen.be

Abstract. Using the Microdosimetric d(z) Model in combination with PHITS-simulated specific energy probability density distributions, the relative efficiency of $^7$LiF:Mg,Ti (MTS) and $^7$LiF:Mg,Cu,P (MCP-7) thermoluminescent detectors was assessed as function of the incident energy for electrons and positrons spanning from 2 keV to 1 GeV. Additionally, the effect of the dopant concentration on the determined efficiency values was carefully investigated. Finally, the results are presented in combination with calculated specific energy frequency mean values and possible correlations were discussed.

1. Introduction
Because of the diverse microscopic pattern of energy deposition induced by different radiation qualities, local phenomena such as saturation of trapping and recombination centres affect strongly the response of luminescent detectors. All of this translates in a reduced or increased luminescence efficiency depending on both the type of particle and its linear energy transfer (LET). For a correct understanding of the data gathered with this type of detectors, their expected response should be well-known for a broad energy-particle spectrum. However, due to time and experimental limitations, a full characterization is not always achievable through exposures in calibrated radiation fields.

Alternatively, by using the recently developed Microdosimetric d(z) Model [1, 2], it is possible to describe and predict these changes in the detector’s response by analysing the stochastic energy deposition at the nanoscale. The model has been employed and successfully benchmarked against experimental data for calculating the relative efficiency of $^7$LiF:Mg,Ti (MTS-7) and $^7$LiF:Mg,Cu,P (MCP-7) thermoluminescent detectors in case of monoenergetic ions from $^1$H to $^{132}$Xe [2], photons [3], and the not-monochromatic radiation field generated by a clinical proton beam [4]. Furthermore, based on the model’s results, a methodology to assess average LET quantities for modelling the relative biological effectiveness (RBE) in clinical proton therapy has been proposed and validated against Monte Carlo simulation and radiobiological experiments [5, 6], underlying further the model’s reliability.

In this paper, we apply the Microdosimetric d(z) Model for calculating the relative efficiency of the two aforementioned detector types in case of monoenergetic electron and positron beams with energy between 2 keV and 1 GeV. The results can be used in order to better understand or correct the results of experimental measurements performed in radiation fields encompassing electrons and positrons.
2. Methodology

Because of inherent difficulties in evaluating an absolute efficiency, the relative luminescence efficiency $\eta_{\text{rel}}$ is generally used to quantify the changes in the detector’s response. This quantity is defined as in Equation 1 as the ratio between the intensity of the luminescent signal $S$ per unit of dose $D$ for the radiation under investigation and a reference one. According to the formalism of the Microdosimetric $d(z)$ Model, the relative luminescence efficiency can be calculated (Equation 1) by folding a detector-specific radiation-independent response function $r(z)$ [1, 2] into the simulated specific energy probability density distribution $d(z)$ for both the radiation under investigation and a reference one. As done in our previous work, the reference radiation was chosen to be the $\gamma$-rays emitted by a $^{60}$Co source.

$$\eta_{\text{rel}} = \frac{\langle S/D \rangle_{\text{radiation under study}}}{\langle S/D \rangle_{\text{reference radiation}}} = \frac{\left[ \int_{0}^{+\infty} d(z) r(z) \, dz \right]_{\text{radiation under study}}}{\left[ \int_{0}^{+\infty} d(z) r(z) \, dz \right]_{\text{reference radiation}}} \quad (1)$$

The specific energy density probability distributions needed for the efficiency calculations with the Microdosimetric $d(z)$ Model were assessed using the [T-SED] tally implemented in the radiation transport code PHITS version 3.16 [7]. The optimal site size of 40 nm was employed for both detector types [1, 2, 3]. Monoenergetic electron and positron beams (energy = 0.002, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, 50, 100, 200, 500, 1000 MeV, diameter = 9 mm) were used to irradiate a simulated detector (cylinder, diameter = 4.5 mm, thickness = 0.9 mm). A dual-energy (1173.2 and 1332.5 keV) photon beam was employed for simulating the reference $^{60}$Co $\gamma$-ray source. The beam direction was orthogonal to the base of the cylinder. In order to investigate the effect of the presence of the dopants on the computed efficiency values, all simulations were performed in pure $^7$lithium fluoride (density = 2.5 g/cm$^3$) and repeated including the nominal dopant atomic concentrations of $^7$LiF:Mg,Ti (MTS-7, Mg=0.0013%, Ti=0.012%) and $^7$LiF:Mg,Cu,P (MCP-7, Mg=0.2%, P=1.25%, Cu=0.05%) thermoluminescent detectors [8]. A total number of $10^7$ particles was used in each run to achieve a statistical uncertainty of all simulated quantities below 0.1%. The cutoff energy of all particles was set to 1 keV/u. The Electron Gamma Shower version 5 (EGS5) code implemented in PHITS was employed to simulate the transport of electrons and positrons. The specific energy distributions were scored in a logarithmic binning from $10^{-4}$ to $10^{8}$ Gy using 50 bins per decades. The minimum energy deposition event considered in the modelling approach is the one relative to one event of one ionization only, leading to an approximate specific energy value of 50 Gy in a 40 nm lithium fluoride target. More details can be found in [1, 2, 3]. Finally, the frequency mean specific energy $\bar{z}_F$ was assessed using Equation 2, where $f(z)$ represents the frequency probability density of the specific energy.

$$\bar{z}_F = \int_{0}^{+\infty} z f(z) \, dz \quad (2)$$

3. Results

In Figure 1 the relative luminescence efficiency of $^7$LiF:Mg,Ti (MTS-7) and $^7$LiF:Mg,Cu,P (MCP-7) thermoluminescent detectors is plotted as function of the incident electron and positron energy. As it can be immediately seen, no relevant differences were found between the results of the Microdosimetric $d(z)$ Model’s calculations between simulations performed including or not the nominal dopant concentrations of both types of detectors. The relative deviation between the two series of values (with or without dopants) was found to be below 0.1% for all particle-energy-detector combinations. The latter value is comparable with the statistical uncertainty of the Monte Carlo calculations.

The calculated efficiency of $^7$LiF:Mg,Ti (MTS-7) is very flat and close to unity ($100 \pm 2\%$) over the whole energy range for both types of particles. On the other hand, the efficiency of $^7$LiF:Mg,Cu,P (MCP-7) detectors for measuring electrons can be subdivided in three regions of interest. In case of electrons energies between 1 and 1000 MeV, the efficiency is very close to 1. For energies between 1 MeV and 20 keV, an efficiency decrease from 1 to 0.7 is observed with the decrease of the incident energy. At lower electron energies, the relative efficiency shows an almost constant value of...
approximately 0.7. The experimental efficiency data points present in literature [9, 10] are included in Figure 1, being in good agreement with the theoretically derived values for both detector types. The efficiency of $^7$LiF:Mg,Cu,P (MCP-7) detectors in case of positrons shows a very similar behaviour to the one for electrons for energies above 20 keV. Nevertheless, the efficiency decrease between 1 MeV and 20 keV positrons is less sharp, reaching a value of 0.76 instead of 0.7. On the other hand, an increase of the efficiency with the decrease of the energy was observed between 20 and 2 keV, for which an efficiency value of 0.87 is predicted. It worth remembering that the combined uncertainty in the calculated efficiency values (deriving from determination of both the response function and the optimal site size of 40 nm) can considered being roughly 10% [1, 2].

Figure 1. Calculated relative luminescence efficiency of $^7$LiF:Mg,Ti (MTS-7) and $^7$LiF:Mg,Cu,P (MCP-7) thermoluminescent detectors plotted as function of the incident energy for monoenergetic electron (left) and positron (right) beams. The simulations were performed both in pure 7lithium fluoride (no dopants) or by including the corresponding nominal dopant concentrations (with dopants). Experimental data from [9, 10] are included for comparison.

Figure 2. Frequency mean specific energy in lithium fluoride as function of the incident electron and positron energy

Figure 3. Response functions of LiF:Mg,Ti (MTS) and LiF:Mg,Cu,P (MCP) detectors as implemented in the Microdosimetric d(z) Model.

In order to better understand the reason between these efficiency changes, Figure 2 shows the calculated fluence mean specific energy in lithium fluoride as function of the energy for both types of particles. No differences (relative deviation < 0.1%) were found between the results of simulations performed in pure
\(^7\)lithium fluoride or by including the nominal concentrations of both types of the detectors. For clarity, only values relative to \(^7\)lithium fluoride are plotted in Figure 2. For both electrons and positrons, \(Z_F\) was found to vary between approximately 240 and 400 Gy, with no differences between the two particles for energies above 100 keV. As it can be seen from Figure 3, the response function of LiF:Mg,Ti (MTS) detectors \([1, 2]\) is flat in this specific energy range (240-400 Gy), explaining the almost unchanged efficiency values calculated for both particle types. On the other hand, for specific energy values above 1 Gy, the response function of LiF:Mg,Cu,P (MCP) detectors \([1, 2]\) shows a decreasing trend with the increase of the specific energy. As a consequence, an almost perfect anti-correlation between calculated LiF:Mg,Cu,P (MCP) efficiency values (Figure 1) and the frequency mean specific energy (Figure 2) is observed for both particles.

4. Conclusions

The relative luminescence efficiency of the two most common thermoluminescent detectors (\(^7\)LiF:Mg,Ti and \(^7\)LiF:Mg,Cu,P) was calculated as function of the incident energy (2 keV – 1 GeV) for monoenergetic electron and positron beams. While the efficiency of the first type of detector was found to be not affected by variations in both energy and the particle (relative efficiency ranging between 0.98 and 1.02), relevant changes were found for \(^7\)LiF:Mg,Cu,P (MCP-7) detectors. In the latter case, the efficiency was found to vary from between 0.7 and 1.03 depending on both the particle type and its energy. Finally, as previously reported in case of Microdosimetric \(d(z)\) Model calculations for ions and photons, the inclusion or exclusion of the nominal dopant concentrations in the simulations was found to play no effect in the computation of the relative efficiency, with variations smaller than 0.1%.

5. References

[1] Parisi A 2018. *Space and Hadron Therapy with Luminescent Detectors: Microdosimetric Modeling and Experimental Measurements*. PhD Thesis, Polytech of Mons
[2] Parisi A 2018 *Rad. Meas.* **123** 1-12
[3] Parisi A 2019 *Rad. Phys. Chem.* **163** 67-73
[4] Parisi A 2020 *Rad. Meas.* (accepted for publication)
[5] Parisi A 2019 *Phys. Med. Biol.* **64** 085005
[6] Parisi A 2020 *Phys. Med. Biol.* **65** 015008
[7] Sato T 2018 *J. Nuc. Sci. Tech.* **55** 684-90
[8] Bilski P 2002 *Radiat. Protect. Dosim.* **100** 199-205
[9] Mobit P N 1996 *Phys. Med. Biol.* **41** 979
[10] Bilski P 1994 *Radiat. Protect. Dosim.* **55** 31-8