CHARACTERIZATION AND MODELING OF RELATIVE LUMINESCENCE EFFICIENCY OF OPTICALLY STIMULATED LUMINESCENCE DETECTORS EXPOSED TO HEAVY CHARGED PARTICLES

By

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8.5 Comparison between OSL $\eta_{HCP,\gamma}$ experimental data and modeling using the RDD functions from Kiefer and Straaten, and Geiß et al. models. The figures in the left side present the comparison for OSL detected with Hoya U-340 filters (F-center and UV emission bands), and the figures in the right side for OSL detected with Hoya U-340 and Schott WG-360 (F-center emission band).

8.6 RDD in Al$_2$O$_3$:C according to the modified version of Butts and Katz model. The RDD was plotted for two different detection windows. For comparison we included the Butts and Katz RDD.

8.7 Comparison between $\eta_{HCP,\gamma}$ experimental data and modeling using the RDD functions from a modified version of Butts and Katz model. The arrows indicate the data points used to find the parameters $A$ and $B$ for the core radius. The insets represent the percentage deviation between data and model. a) OSL from Luxel$^{TM}$ detected with Hoya U-340 filters (F-center and UV emission bands); b) OSL from Luxel$^{TM}$ detected with Hoya U-340 and Schott WG-360 (F-center emission band).

8.8 Comparison between $\eta_{HCP,\gamma}$ experimental data and modeling using the RDD functions from a modified version of Butts and Katz model. The experimental data was obtained by placing binary filters in front of the H 40 MeV, He 150 MeV/u, Ne 400 MeV/u, and Si 490 MeV/u to stop the primary particles. The full lines represent the results from the modeling, and symbols the experimental data. The insets represent the percentage deviation between data and model. a) OSL from Luxel$^{TM}$ detected with Hoya U-340 filter (F-center and UV emission bands); b) OSL from Luxel$^{TM}$ detected with Hoya U-340 and Schott WG-360 filters (F-center emission band).

8.9 Influence of the thickness $z$ of the detector on the $\eta_{HCP,\gamma}$ calculated in water using GEANT4. The dashed lines represent the interval of the experimental data for one standard deviation of the data.
8.10 Relative luminescence efficiency versus $L_\infty$ in water using RDD simulated with GEANT4 for different detector thicknesses $z$. a)-c) $\eta_{HCP,\gamma}$ when OSL from Luxel™ is detected with Hoya U-340 filter (F-center emission band). d)-f) $\eta_{HCP,\gamma}$ when OSL from Luxel™ is detected with Hoya U-340 and Schott WG-360 filters (F-center emission band).

9.1 Method to estimate the “effective” LET $L_{\infty}^{eff}$, and effective relative luminescence efficiency $\eta_{HCP,\gamma}^{eff}$ of the radiation field using OSL from Luxel™. a) Characterization of the shape of the OSL curve from Luxel™ to different LETs. The ordinate axis represents the “Ratio” between the OSL initial intensity and total area. b) Relative luminescence efficiency as a function of LET. The OSL was measured with Hoya U-340 filters detecting F-center and UV emission bands. The red lines are arbitrary functions fitted to the data for better visualization.

A.1 $\eta_{HCP,\gamma}$ calculated in water of OSL from Al₂O₃:C single crystal detectors. We considered the OSL signal equal to the total area under the OSL curve. The OSL was measured with Hoya U-340 filter detecting both F-center and UV emission bands. For comparison we include the Luxel™ data (full and dashed lines).

A.2 $\eta_{HCP,\gamma}$ calculated in water of TL from Al₂O₃:C single crystal detectors. We considered the TL signal equal to the height of the dosimetric TL peak. The TL was measured with Corning 5-58 filter detecting both F-center emission band. For comparison we include the Luxel™ data (full and dashed lines).

A.3 $\eta_{HCP,\gamma}$ calculated in water of TL from TLD-100 detectors. We considered the TL signal equal to the height of the dosimetric TL peak. The TL was measured with Schott BG-39 filter. For comparison we include the Luxel™ data (full and dashed lines).
NOMENCLATURE

**BNL**  Brookhaven National Laboratory

**CW-OSL**  Continuous-Wave Optically Stimulated Luminescence

**DDCS**  Double Differential Cross-Section

**DET**  Deep Electron Trap

**DHT**  Deep Hole Trap

**FWHM**  Full Width at Half Maximum

**HCP**  Heavy Charged Particle

**HIMAC**  Heavy Ion Medical Accelerator in Chiba

**ICCHIBAN**  Inter-Comparison for Cosmic-rays with Heavy Ion Beams at NIRS

**ICRU**  International Commission on Radiation Units and Measurements

**LED**  Light Emitting Diode

**LET**  Linear Energy Transfer

**LLUMC**  Loma Linda University Medical Center

**LM-OSL**  Linear-Modulation Optically Stimulated Luminescence

**MC**  Monte Carlo

**MDT**  Main Dosimetric Trap
NIRS  National Institute of Radiological Sciences

NIST  National Institute of Standards and Technology

NSRL  NASA Space Radiation Laboratory

OSL   Optically Stimulated Luminescence

OSLD  Optically Stimulated Luminescence Dosimeter/Detector

OSU   Oklahoma State University

PNTD  Plastic Nuclear Track Detector

POSL  Pulsed Optically Stimulated Luminescence

RDD  Radial Dose Distribution

SDCS  Single Differential Cross-Section

TAMU  Texas A & M University

TL    Thermoluminescence

TLD   Thermoluminescence Dosimeter/Detector

TSM   Track Structure Model

UV    Ultraviolet
LIST OF SYMBOLS

$A$ re-trapping probability of electrons

$A_m$ recombination probability of electrons with holes

$c$ speed of light in vacuum

$D(r)$ radial dose distribution

$D_k$ absorbed dose from a radiation field $k$

$e$ electron charge

$E_k$ energy imparted from a radiation field $k$

$f_k$ response function from a detector exposed to the radiation field $k$

$I$ ionization potential

$I_0$ optically stimulated luminescence initial intensity

$I_{OSL}$ optically stimulated luminescence intensity

$L$ maximum depth of penetration

$L_m^\infty$ unrestricted linear energy transfer calculated in the material $m$

$m$ concentration of holes in the hole trap

$m_e$ electron mass

$m_v$ concentration of holes in the valence band

$m_e c^2$ rest energy of an electron

$N_e$ density of electrons

$N$ total concentration of electron traps

$n$ concentration of electron in the electron trap

$n_c$ concentration of electron in the conduction band
$n_k$ concentration of low energy charges created by the radiation field $k$

$r$ radial distance

$r_c$ core radius

$R_{Max}$ penumbra radius

$S_k$ luminescence signal produced by the radiation field $k$

$t$ time

$V$ volume

$W$ maximum energy of secondary electrons in a heavy charged particle collision

$W_k$ average energy required to create an electron-hole pair by the radiation field $k$

$w$ electron energy

$Z$ atomic number

$Z^*$ effective atomic number

$\alpha$ detection efficiency of the experimental apparatus

$\beta$ relative velocity with respect to velocity of light in vacuum

$\eta_k$ luminescence efficiency to the radiation field $k$

$\eta'_k$ efficiency to convert low energy charges created by the radiation field $k$ into luminescence

$\eta_{k,l}$ relative luminescence efficiency of radiation field $k$ in respect with a reference radiation field $l$

$\rho_m$ density of the medium

$\sigma$ photoionization cross-section

$\tau_d$ optically stimulated luminescence decay constant

$\Phi$ fluence

$\Omega_p$ plasma oscillation frequency
CHAPTER 1

INTRODUCTION

This work investigates the optically stimulated luminescence (OSL) response of carbon-doped aluminum oxide (Al$_2$O$_3$:C) detectors exposed to heavy charged particles (HCPs) with energies relevant to radiation protection in space, and cancer therapy. This investigation includes ground-based experiments in accelerators and theoretical studies of the detector’s response. These theoretical studies are based on the track structure model (TSM) and require information of the spatial pattern of energy deposition around the HCP path – the radial dose distribution (RDD). Thus, RDDs were obtained using six analytical models, and Monte Carlo simulations with the code GEANT4. In addition, we propose a modified analytical model to improve the agreement between calculated and experimental efficiency values.

The interest in HCP$^1$ dosimetry is growing because of the increasing human presence in space geared toward future manned space exploration missions, and the dissemination of new facilities for proton and carbon cancer therapy. However, the dosimetry of HCPs remains a challenging problem in luminescence dosimetry, motivating the investigation of the effects of HCPs on new detectors, such as Al$_2$O$_3$:C OSL detectors (OSLDs). For appropriate use of radiation and for radiation protection, development of new dosimetric methods is important for reliable measurement of absorbed doses in HCP radiation fields.

The challenge in space dosimetry stems from the presence of different particles with a wide range of energies (McKeever, 2002; Benton and Benton, 2001). Solid state luminescence detectors exhibit decreasing efficiency with increasing ionization density of the

\footnote{Throughout this work the term heavy charged particle (HCP) is used for all nuclei, including proton.}
radiation field (Horowitz, 1981; Olko, 2002; Yukihara et al., 2006), making the detector’s response dependent upon the spectrum of the radiation field. The decreasing efficiency is due to the non-uniform distribution of physical events created by the HCP along its path, which produces doses as high as $10^6$ Gy (Gy = J/kg) along the vicinity of the track, depending on the charge and speed of the particle (Butts and Katz, 1967). To complicate matters even further, the ionization density is not uniquely related to the linear energy transfer (LET), but depends on the particle atomic number $Z$ and energy $E$ (Horowitz, 1981).

Proton and carbon cancer therapy dosimetry is also challenging because the particle’s energy varies along the Bragg curve, therefore affecting the luminescence efficiency. In addition, in proton and carbon therapy, the energy of the beam is spread using a “range shifter” to create the so-called “spread-out Bragg peak” (Ragu, 1980). Consequently, any point measurement of the dose includes contributions from particles with different energies.

OSL is a technique of growing importance in HCP dosimetry. In addition to the advantages common to solid state luminescence detectors, such as small size, no need for power or cables, and no power consumption, Al$_2$O$_3$:Cr OSLDs also offer high sensitivity, rapid readout, elimination of complex thermal annealing steps, possibility of re-estimation of absorbed dose, possibility of dose imaging, high precision, and accuracy (McKeever and Moscovitch, 2003; Yukihara et al., 2006). In personnel dosimetry in space, the partial solution to the HCP dosimetry problem is to combine two or more types of detectors with complementary properties, such as thermoluminescence (TL) detectors (TLDs) or OSLDs, and plastic nuclear track detectors (PNTD) (NCRP, 2002; McKeever et al., 2007). TLDs and OSLDs are efficient for low LET radiation (LET in water, $L_{\infty}^{H_2O} < 10$ keV/µm), whereas PNTDs are efficient for high LET radiation ($L_{\infty}^{H_2O} > 10$ keV/µm). Al$_2$O$_3$:Cr OSLDs are currently part of the NASA crew and area monitoring detector packages (Zhou et al., 2006, 2007), and are also under investigation for real-time in vivo proton therapy dosimetry (Edmund et al., 2007b,a).

The objective of this work is to evaluate the possibility of applying the TSM to predict
the response of luminescence detectors to different combinations of HCPs and energies relevant to radiation protection in space and cancer therapy. Such a model is important considering that only a limited number of accelerator facilities around the world can provide the relevant combination of HCPs and energies for characterization of the detectors. Therefore, the experimental characterization is very time consuming and expensive.

This work will be presented according to the following structure.

Chapters 2 to 5 present the theoretical background and calculations of RDDs. The basic properties and model for the OSL are presented in chapter 2, which provides the basis to understand the results of this dissertation. Chapter 3 derives a formula to predict the relative luminescence efficiency ($\eta_{HCP,\gamma}$) of detectors exposed to HCPs. The formula requires RDDs that are obtained in chapters 4 and 5 using analytical models and Monte Carlo simulations.

Chapters 6 and 7 present the experimental work on the characterization of luminescence detectors. The experimental details (type of detectors, measurement, HCP irradiations, and protocols) are presented in chapter 6, whereas experimental results on the OSL dose response, shape of the OSL curve, and $\eta_{HCP,\gamma}$ data for different types of radiation are presented in chapter 7. A complete table with $\eta_{HCP,\gamma}$ data for different detector’s type (Luxel\textsuperscript{TM}, Al\textsubscript{2}O\textsubscript{3}:C single crystal and TLD-100), readout method (OSL and TL), and combinations of HCPs and energies can be found in the Appendix A.

Chapters 8 and 9 combine the theoretical background with the experimental results. The predictions of the OSL response of Luxel\textsuperscript{TM} detectors are compared with experimental data in chapter 8. In addition to the analytical models of RDD presented in chapter 4, we propose a modified model which predicts relative luminescence efficiency values for Luxel\textsuperscript{TM} detectors in agreement with experimental data within 20%. Moreover, the relative luminescence efficiencies predicted with the Monte Carlo code GEANT4 are compared with experimental data. Additionally, chapter 9 discusses a method to measure absorbed dose and dose equivalent in space, which incorporates the results of this dissertation.
To conclude, chapter 10 summarizes the relevant results, discusses the limitations and weaknesses of our approach, and suggests improvements and future work.
CHAPTER 2

OPTICALLY STIMULATED LUMINESCENCE

Optically stimulated luminescence (OSL) is a phenomenon of light emission by an irradiated insulator or semiconductor crystal when the material is exposed to light of appropriate wavelength. Synthetic $\text{Al}_2\text{O}_3$:C crystal is one of the most sensitive OSL materials, being used for personnel, environmental, and medical dosimetry applications on Earth (Bøtter-Jensen et al., 2003), and for crew passive and area monitoring in space (Zhou et al., 2006, 2007). This chapter presents the basic theoretical framework of OSL and a summary of the luminescence properties and characteristics of $\text{Al}_2\text{O}_3$:C material that are relevant to understand the results of this dissertation.

2.1 THE OPTICALLY STIMULATED LUMINESCENCE PHENOMENON

The OSL intensity, also called OSL signal, is proportional to the energy absorbed by the detector. A band diagram containing two localized pre-existing defects between the conduction and valence bands summarizes the OSL process. Defects localized between the bottom of the conduction band and Fermi level, called electron traps, can localize free electrons moving in the conduction band. On the other hand, defects localized between the top of the valence band and Fermi level, called hole traps, can localize free holes moving in the valence band. The band diagram in Figure 2.1 summarizes the OSL process: i) the material is in the ground state; ii) ionizing radiation creates electron-hole pairs; the free electrons move in the conduction band and free holes in the valence band; pre-existing defects within the material can localize the free electrons and holes; iii) after the irradiation is over the trapped electrons and holes remain in a metastable state; iv) illumination with
an appropriate wavelength leads to electron transitions from the trap into the delocalized conduction band. Recombination of the free electrons with localized holes, (or vice-versa) results in luminescence emission (Bøtter-Jensen et al., 2003).

The OSL curve is a graph of the OSL intensity versus time of stimulation. The OSL curve can be read out under different conditions including continuous-wave OSL (CW-OSL) (Figure 2.2a), linear-modulation OSL (LM-OSL) (Figure 2.2b), and pulsed OSL (POSL) (Figure 2.2c). This work uses the CW-OSL readout. The advantages of each readout mode are discussed in Bøtter-Jensen et al. (2003).

The simplest OSL model is a crystal containing only one type of electron trap and one type of hole trap participating in the luminescence process (Figure 2.1). In this case, when the stimulation light is turned on, trapped electrons are excited to the conduction band with

Figure 2.1: Band diagram illustrating the OSL phenomenon. Full and empty circles represent electrons and holes, respectively. \( E_e \) and \( E_h \) are the activation energies of the electron trap and hole trap, respectively.

\[ \begin{align*}
\text{i) Ground state} \\
\text{Conduction band} \\
\text{Electron trap} \\
\text{Fermi level} \\
\text{Hole trap} \\
\text{Valence band} \\
\text{ii) Irradiation} \\
\text{iii) Metastable state} \\
\text{iv) Stimulation} \\
\text{OSL} \\
\end{align*} \]
Figure 2.2: Examples of OSL curves obtained with three readout methods: (a) CW-OSL, (b) LM-OSL and (c) POSL. The insets represent the stimulation power as a function of time (courtesy of E. G. Yukihiro).
probability rate \( p \). The probability rate \( p \) is equal to the incident photon flux \( \Phi \) times the photoionization cross-section \( \sigma \) \( (p = \Phi \sigma) \). The electrons in the conduction band can be re-trapped by the electron traps with probability \( A \), or recombine with a hole in a hole trap, also called recombination center, with probability \( A_m \). The electron-hole recombination at the recombination center follows OSL emission. Charge neutrality for this system can be written as

\[
    n_c + n = m_v + m
\]

(2.1)

where \( n_c \) and \( n \) are the concentrations of electrons in the conduction band and electron traps, respectively, and \( m_v \) and \( m \) are the concentrations of holes in the valence band and hole traps, respectively.

Considering that at the beginning of the optical stimulation \( n_c = m_v = 0 \), then \( n_0 = m_0 \). The subscript 0 stands for time \( t = 0 \).

Assuming that optical stimulation only causes electron transitions to the conduction band, the rate of change in the concentrations can be written as

\[
    \frac{dn_c}{dt} = -\frac{dn}{dt} + \frac{dm}{dt}
\]

(2.2)

where

\[
    \frac{dn}{dt} = -np + n_cA(N - n)
\]

(2.3)

and

\[
    \frac{dm}{dt} = -n_cA_mm
\]

(2.4)

where \( N \) is the total available concentration of electron traps. Considering that the rate of change in the concentration of electrons in the conduction band is low compared to the rate of change in the traps (the so called “quasi-equilibrium approximation”), \( dn_c/dt \ll
\( \frac{dn}{dt}, \frac{dm}{dt} \) and \( n_c \ll n, m \), we have from 2.2 that:

\[
\frac{dm}{dt} = \frac{dn}{dt} \tag{2.5}
\]

Assuming that there is slow re-trapping of electrons, \( n_c A (N - n) \ll np, n_c A m m \). Thus, the OSL intensity as a function of time can be written as

\[
I_{\text{OSL}}(t) = -\frac{dm}{dt} = -\frac{dn}{dt} = np \tag{2.6}
\]

in which the solution is a pure exponential decay

\[
I_{\text{OSL}}(t) = n_0 p e^{-tp} = I_0 e^{-\frac{t}{\tau_d}} \tag{2.7}
\]

where \( I_0 \) is the initial OSL intensity at \( t = 0 \) and \( \tau_d = 1/p \) is the OSL decay constant. Thus, the simplest model of only one type of electron trap and one type of recombination center leads to a OSL intensity that decays exponentially as the constant stimulation light intensity is applied to the sample (Bøtter-Jensen et al., 2003).

### 2.2 Optically Stimulated Luminescence Properties of Al\(_2\)O\(_3\):C

Al\(_2\)O\(_3\):C, first introduced as a TLD (Akselrod et al., 1990, 1993), has been widely used as an OSLD over the last decade. The high sensitivity, fast and all-optical nature of OSL readout of Al\(_2\)O\(_3\):C opened the possibility of developing new technologies such as: POSL (McKeever et al., 1996; McKeever and Akselrod, 1999), imaging (Akselrod et al., 2000), and remote real-time fiber dosimetry (Huston et al., 2001; Polf et al., 2002; Aznar et al., 2004). These technologies have been used in environmental (Kalchgruber and Wagner, 2006), personnel, medical (Aznar et al., 2004, 2005; Andersen et al., 2006), and space dosimetry (Goossens et al., 2006; Yukihara et al., 2006).

Figure 2.3 presents a band diagram model that summarizes the OSL process in Al\(_2\)O\(_3\):C
(Yukihara et al., 2004b; Yukihara and McKeever, 2006a; Chen et al., 2006; Pagonis et al., 2006). Because the defects participating in the OSL, thermoluminescence (TL) and radioluminescence (RL) processes are the same, the band diagram also explains these phenomena (Bøtter-Jensen et al., 2003).

The defects relevant to the OSL process in Al$_2$O$_3$:C are the main dosimetric trap (MDT) and oxygen vacancies. The nature of the MDT is unclear (Yukihara and McKeever, 2006a), although the MDT is usually considered to be an electron trap (Bøtter-Jensen et al., 2003). Al$_2$O$_3$:C crystals are grown with a high concentration of oxygen vacancies. The oxygen vacancies with two captured electrons (F-center) and one captured electron (F$^+$-center) are the most important. Radiative relaxation of the F-centers is responsible for the main luminescence emission at $\sim$ 420 nm (Evans and Stapelbroek, 1978; Evans et al., 1994).

![Band diagram model of the main defects involved in the OSL, TL and RL in Al$_2$O$_3$:C.](image)

Figure 2.3: Band diagram model of the main defects involved in the OSL, TL and RL in Al$_2$O$_3$:C. The numbers indicate the possible electronic transitions during the irradiation stage. MDT, DET and DHT stand for main dosimetric trap, deep electron trap and deep hole trap, respectively (Yukihara et al., 2004b; Yukihara and McKeever, 2006a; Chen et al., 2006; Pagonis et al., 2006).

We summarize the filling of traps in Al$_2$O$_3$:C during radiation as follows: ionizing radiation creates electron-hole pairs in the conduction band and valence band of the crystal. When the electrons are in the conduction band they are free to move and they can be trapped in the MDT, deep electron traps (DET), or undergo recombination with F$^+$-centers.
Recombination of electrons with F$^+$-centers produces F-centers in the excited state

$$F^+ + e^- \rightarrow F^*$$ \hspace{1cm} (2.8)

Then, F-center transitions to the ground state causes luminescence emission at 420 nm

$$F^* \rightarrow F + h\nu_{420\text{nm}}$$ \hspace{1cm} (2.9)

On the other hand, free holes can be trapped at deep hole traps (DHT) and F-centers. The trapping of holes in F-centers causes F-center to F$^+$-center conversion:

$$F + h^+ \rightarrow F^+$$ \hspace{1cm} (2.10)

During the OSL or TL readout, electrons are released from the MDT and recombine with the F$^+$-centers resulting in luminescence emission at 420 nm (eqs. 2.8 and 2.9).

Step annealing studies of the F$^+$-center optical absorption band in irradiated and ultraviolet (UV) illuminated Al$_2$O$_3$;C crystals confirmed the existence of DET and DHT (Akselrod and Gorelova, 1993; Yukihara et al., 2003, 2004b). Heating irradiated crystals to (500-600) °C causes an increasing in the F$^+$-center optical absorption band. This increasing is due to the release of holes from deep traps unstable in this temperature range, and creation of F$^+$-centers (see eq. 2.10). The evidence of DET is a decrease in the F$^+$-center optical absorption band at $\sim$ (700-1000) °C, attributed to the releasing of electrons from deep traps and conversion of F$^+$-centers to F-centers (see eq. 2.8). Changes in the concentration of F$^+$-centers cause changes in the sensitivity of the material. Annealing to 900 °C empties the DET and DHT restoring the sensitivity of the crystal (Yukihara et al., 2004b).

The model presented in Figure 2.3 is a simplification of the OSL process in Al$_2$O$_3$;C. In fact, other defects participate in the OSL emission. For example, the model ignores the presence of an unknown defect responsible for an emission band centered at $\sim$ 334 nm
Figure 2.4: OSL emission spectrum of Al$_2$O$_3$:C samples irradiated with 200 Gy of $^{60}$Co gamma rays during short stimulation pulses of 500 ns (Yukihara and McKeever, 2006b). (Yukihara and McKeever, 2006b) (Figure 2.4). Taking advantage of the short lifetime of the UV emission band ($< 6 \mu s$) (Evans and Stapelbroek, 1978; Yukihara and McKeever, 2006b) compared to the F-center emission band (35 ms) (Lee and Crawford, 1979; Markey et al., 1995), Yukihara and McKeever (2006b) used time discrimination OSL to study the dependence of the F-center and UV emission bands to ionization density. Yukihara and McKeever (2006b) observed that the contribution of OSL from the UV emission band to the total OSL emission increases as the ionization density increases. Furthermore, the intensity of the UV emission band at room temperature increases with time elapsed since irradiation. Such observations are important when applying the Al$_2$O$_3$:C OSL to HCP radiation because HCPs create high ionization densities in the vicinity of their paths. Thus, adequate readout procedures with detection of the appropriate luminescence bands are important.
CHAPTER 3

RESPONSE OF LUMINESCENCE DETECTORS TO HEAVY CHARGED PARTICLE RADIATION

Heavy charged particles (HCPs) dissipate energy in matter mainly through electromagnetic interactions with the atoms of the material. The main product of the electromagnetic interactions are ionizations and excitations of the medium for HCPs with energies greater than $\sim$ 0.1 MeV/u (Kalef-Ezra and Horowitz, 1982; ICRU, 1993). Excitations deposit energy locally, whereas ionizations produce secondary electrons (delta rays). The secondary electrons can deposit energy at large distances from the path of the particle. Thus, the passage of HCP through matter leaves a trail of physical events characterized by the HCP’s atomic number and speed. The spatial distribution of the physical events created around the HCP path, the radial dose distribution (RDD), influences the final effect produced by the radiation action (e.g. OSL, TL, mutation inductions, DNA strand breaks, etc).

Figure 3.1 illustrates this spatial distribution of the physical events created around the path of He 144.2 MeV/u and Fe 120.4 MeV/u particles in water. Figure 3.1 was created using the Monte Carlo code GEANT4 (Agostinelli et al., 2003). The number of incident particles is the same for both simulations. Figure 3.1 shows that the Fe 120.4 MeV/u particle produces higher ionization densities than the He 144.2 MeV/u particle. The distribution of secondary particles (red lines) produced by ionizations of the medium is a characteristic of the particle’s atomic number and speed. In regions close to the path of the HCP the local absorbed dose reaches values as large as $10^6$ Gy, depending on the HCP’s charge and speed. Therefore, in regions of such high localized doses, the traps responsible for the luminescence process may become totally filled, saturating the detector. Moreover, for the energies
of HCPs relevant to this work, secondary particles that deposit energy in the material can have energies as low as a few eV, and as high as a few MeV.

Figure 3.1: Monte Carlo simulations with GEANT4 of He and Fe tracks in water. The number of primary particles in both simulations is the same. The blue line is the primary particle, red lines are negative charged secondary, tertiary and higher order particles, and the yellow dots are interaction points where events occurred.

Due to the different ionization density profiles, we expect the response of luminescence detectors to vary for different types of HCP radiation. Indeed, the literature documents the experimental dependence of the relative luminescence efficiency to HCP ($\eta_{HCP,\gamma}$) (see section 3.1).

The definition of efficiency of a luminescence detector to a radiation field $k$ is the ratio between the energy emitted by the detector as luminescence $\epsilon_k$ and the mean absorbed energy $E_k$ by the detector from the radiation field $k$:

$$\eta_k(E_k) = \frac{\epsilon_k(E_k)}{E_k} \quad (3.1)$$

The energy emitted as luminescence $\epsilon_k$ relates to the total amount of light collected by
the experimental apparatus $S_k$ through:

$$\epsilon_k(E_k) = \alpha^{-1} S_k(E_k)$$  \hspace{1cm} (3.2)

where $\alpha$ is the detection efficiency of the experimental apparatus, which depends on experimental factors such as quantum efficiency of the light detector, and light collection efficiency.

The definition of the relative luminescence efficiency follows as the ratio of the luminescence efficiency of two radiation fields. Thus, the relative luminescence efficiency of detectors with the same mass to the radiation field $k$ with respect to a reference radiation field $l$, $\eta_{k,l}$, is defined as

$$\eta_{k,l} = \frac{\eta_k(E_k)}{\eta_l(E_l)} = \frac{S_k(E_k)}{E_k} \frac{E_l}{S_l(E_l)}$$  \hspace{1cm} (3.3)

where $E_k$ and $E_l$ are the mean absorbed energy from the radiation fields $k$ and $l$, respectively, and $S_k$ and $S_l$ are the luminescence signals of detectors with the same mass produced by the radiation fields $k$ and $l$, respectively. Measuring both luminescence efficiencies with the same experimental apparatus, the detection efficiency of the experimental apparatus $\alpha$ cancels out.

### 3.1 EXPERIMENTAL RELATIVE LUMINESCENCE EFFICIENCY

Considerable investigation has been performed on the response of luminescence detectors to neutron and HCPs. Experimental results show that detectors exposed to HCP present different luminescence efficiencies compared to detectors exposed to $^{60}$Co gamma radiation (Horowitz, 1981). To quantify the different responses of the detectors for intercalibration purposes, investigators established the relative luminescence efficiency, $\eta_{\text{HCP},\gamma}$, versus unrestricted linear energy transfer ($L_\infty$), as a parameter to characterize the response.
of the detectors to different particles and energies. Horowitz (1981) presents a compilation of $\eta_{\text{HCP},\gamma}$ versus $L_\infty$ data for LiF, Li$_2$B$_4$O$_7$:Mn, and CaF$_2$:Mn TL materials (see Figure 3.2 for LiF). The TL data show a general trend of decreasing the $\eta_{\text{HCP},\gamma}$ for increasing LET of the radiation field.

Figure 3.2: Relative luminescence efficiency, $\eta_{\text{HCP},\gamma}$, versus unrestricted linear energy transfer, $L_\infty$, of LiF. The ordinate axis refers to the relative luminescence efficiency of HCP relative to gamma radiation (see eq. 3.3) and the abscissa axis refers to the unrestricted linear energy transfer in units of mass stopping power. The data is a compilation of different experiments performed by different groups. Horowitz (1981) provides the references listed in the figure.

Data on the OSL $\eta_{\text{HCP},\gamma}$ of Al$_2$O$_3$:C show the same general trend of decreasing the $\eta_{\text{HCP},\gamma}$ for increasing LET of the radiation field (Figure 3.3) (Yasuda et al., 2002; Yukihara et al., 2004a; Gaza et al., 2004; Gaza, 2004).
Figure 3.3: OSL $\eta_{HCP,\gamma}$ versus $L^H_{\infty}$ of Luxel™ detectors ($Al_2O_3:C$). The OSL signal was considered to be the total area under the OSL curve. The data is a compilation of all experiments performed at Oklahoma State University before this work (Gaza, 2004).

### 3.2 TRACK STRUCTURE MODEL

For the last 40 years semi-empirical models have been used to predict the response of different systems to HCP radiation. The track structure model (TSM) (Butts and Katz, 1967) and microdosimetric model (Rossi and Zaider, 1996) compare the biological efficiency of different HCP radiations using biological end-points relevant to radiation protection (mutation inductions, chromosome aberrations, DNA strand breaks), or radiotherapy (cell survival). The TSM and microdosimetry also provide the framework to predict the response of detectors, such as TLDs and dye films, to HCPs (Horowitz, 1981; Kalef-Ezra and Horowitz, 1982; Katz et al., 1972; Waligórski and Katz, 1980; Hansen and Olsen, 1984; Geiß et al., 1998; Olko, 2002). This section presents the fundamentals of the TSM and derives an expression to predict $\eta_{HCP,\gamma}$ values from knowledge of the RDD and luminescence response of the detector to low LET radiation.
Butts and Katz (1967) introduced the TSM to explain the response of dry enzymes and viruses exposed to HCP. The model’s main hypothesis is that the final effect (such as luminescence, DNA strand breaks and mutation) produced by HCP radiation can be approximated by the bulk effect created by uniform electron or photon radiation of a macroscopic volume (test radiation), so that the processes that take place in the macroscopic volume mimic as closely as possible the processes that take place in the volume element $dV$ under HCP irradiation (Kalef-Ezra and Horowitz, 1982). If the only factor that influences the final effect in a system is the density of ionizations, the final effect can be approximately simulated using electron or photon irradiations. Then, knowledge of the RDD around the HCP path allows the calculation of the final effect of the system under HCP irradiation. Following we present an expression to calculate the $\eta_{HCP,\gamma}$ of detectors based on the TSM. We adopt the Kalef-Ezra and Horowitz (1982) formalism to derive the $\eta_{HCP,\gamma}$ expression.

In luminescence detectors the final effect produced by the HCP radiation is emission of light. Eq. 3.3 gives the relative luminescence efficiency expression. We use gamma rays from a $^{60}$Co source as the reference radiation field because gamma rays from a $^{60}$Co source are one of the standard calibration fields in dosimetry.

Rewriting eq. 3.3 with the appropriated notation we have

$$\eta_{HCP,\gamma} = \frac{S_{HCP}}{E_{HCP}} \frac{S_{\gamma}}{E_{\gamma}}$$

(3.4)

where $S_{HCP}$ and $S_{\gamma}$ are the signals of detectors with the same mass, thickness, and volume created under HCP and gamma radiations, respectively, $E_{HCP}$ is the mean absorbed energy from a HCP beam of fluence $\Phi$ on the detector’s area $A$, and $E_{\gamma}$ is the mean absorbed energy from gamma radiation. For equal doses delivered to the whole detector, $D_{HCP} = D_{\gamma}$. For detectors with the same mass, $E_{HCP} = E_{\gamma}$, and the relative luminescence efficiency is simply $\eta_{HCP,\gamma} = S_{HCP}/S_{\gamma}$.

Kalef-Ezra and Horowitz (1982) consider the luminescence signal as proportional to
the concentration of low energy charges $n_k$ created by the radiation $k$ within the lattice of the crystal. These low energy charges are trapped and converted to luminescence with efficiency $\eta'_k$. Therefore, the luminescence signal of the detector is:

$$S_k = \alpha \eta'_k n_k V$$  \hspace{1cm} (3.5)$$

where the index $k$ indicates the type of radiation, $\alpha$ is the detection efficiency of the experimental apparatus, $\eta'_k$ is the efficiency to convert the low energy charges created by the radiation $k$ into luminescence, and $n_k$ is the concentration of low energy charges created by the radiation $k$.

Figure 3.4 illustrates the difference between the efficiency $\eta'_k$ to convert the low energy charges created by the radiation $k$ into luminescence, and the luminescence efficiency $\eta_k$ (see eq. 3.1).

Figure 3.4: Illustration of the luminescence process. The material’s volume $V$ absorbs the energy $E_k$ from the radiation $k$ creating a concentration of low energy free charges $n_k$. The low energy free charges are trapped in the main dosimetric trap. The trapped charges are proportional to the luminescence signal. $W_k$ is the average energy required to create a electron-hole pair by the radiation $k$.

The absorbed energy $E_k$ is given by:

$$E_k = W_k n_k V$$  \hspace{1cm} (3.6)$$
where $W_k$ is the average energy required to create an electron-hole pair by the radiation $k$, $n_k$ is the concentration of low energy free charges created by the radiation $k$, and $V$ is the irradiated volume.

Thus, we find the relationship between $\eta_k$ and $\eta_k'$ substituting eq. 3.6 and eq. 3.5 in eq. 3.1:

$$\eta_k = \frac{\eta_k'}{W_k} \quad (3.7)$$

The absorbed dose $D_k$ can be obtained as:

$$D_k = \frac{W_k n_k V}{m} = \frac{W_k n_k}{\rho_m} \quad (3.8)$$

where $V$, $m$, and $\rho_m$ are the volume, mass, and density of the detector. Thus, the signal as a function of absorbed dose is given by

$$S_k(D_k) = \alpha \eta_k D_k \rho_m V = \alpha \eta_k D_k \rho_m V \quad (3.9)$$

For convenience we define the luminescence response function or supralinearity index $f_k(D)$ of an uniformly irradiated mass of the luminescence detector to the radiation field $k$ as:

$$f_k(D) = \frac{\eta_k(D)}{\eta_k(D_0)} \quad (3.10)$$

where $\eta_k(D)$ is the luminescence efficiency at absorbed dose $D$ and $\eta_k(D_0)$ is the luminescence efficiency obtained at the “low dose” $D_0$ where the signal $S_k$ is linear.

Figure 3.5 shows an example of the dose response and luminescence response function $f_k(D)$ for a detector that behaves linearly in the “low dose” range followed by saturation.

Thus, for gamma radiation the signal becomes

$$S_{\gamma}(D) = \alpha \eta_{\gamma}(D_0) f_{\gamma}(D) D_{\gamma} \rho_m V \quad (3.11)$$
The mean absorbed energy from gamma rays is given by:

\[ E_\gamma = D_\gamma \rho_m V \]  \hspace{2cm} (3.12)

Therefore, the luminescence efficiency to the gamma radiation field is given by (eq. 3.1)

\[ \eta_\gamma(D) = \frac{\alpha^{-1} S_\gamma}{E_\gamma} = \eta_\gamma(D_0) f_\gamma(D) \]  \hspace{2cm} (3.13)

For HCPs, the signal \( dS_{HCP} \) of an element of volume \( dV \) of a detector exposed to a single HCP can be written differentiating eq. 3.9

\[ dS_{HCP} = \alpha \eta_\delta' \frac{D(r, l)}{W_{HCP}} \rho_m dV = \alpha \eta_\delta D(r, l) \rho_m dV \]  \hspace{2cm} (3.14)

where \( \eta_\delta' \) is the efficiency to convert the low energy charges created by the HCP into luminescence, \( D(r, l) \) is the RDD around the path of the incident HCP, \( W_{HCP} \) is the average energy required to create an electron-hole pair by HCP radiation, and \( \eta_\delta \) is the luminescence efficiency to the delta ray (subscript \( \delta \)) spectrum created by the HCP.
Using eq. 3.10, the signal due to HCP radiation becomes

\[ dS_{HCP} = \alpha \eta_\delta(D_0) f_\delta[D(r, l)] D(r, l) \rho_m dV \]  

(3.15)

where \( \eta_\delta(D_0) \) is the luminescence efficiency to the delta ray (subscript \( \delta \)) spectrum created by the HCP in the “low dose” region of the response of the detector, and \( f_\delta[D(r, l)] \) is the luminescence response function of the detector to the delta rays created by the HCP. Note that \( f_\delta[D(r, l)] \) is a function of the RDD.

Fain et al. (1974) showed that the average energy required to create an ion pair in gas by HCP radiation varies as a function of the radial distance from the path of the incident HCP. Although data on the dependence of \( W_{HCP} \) as a function of radial distance in solids are unavailable, likely the \( W_{HCP} \) in solids presents the same trend. Thus, the luminescence efficiency \( \eta_\delta(D_0) \) changes with radial distance from the path of the HCP. \( W_{HCP} \) data in solids are scarce and exist only for a restricted number of scintillator materials (ICRU, 1979; IAEA, 1995).

A HCP beam with fluence \( \Phi \) incident in the detector area \( A \) produces the luminescence signal \( S_{HCP} \) given by:

\[ S_{HCP} = \Phi \int_0^{R_{Max}} \int_0^L \alpha \eta_\delta(D_0) f_\delta[D(r, l)] D(r, l) \rho_m 2\pi r dr dl \]  

(3.16)

where \( R_{Max} \) is the maximum radial distance of the delta rays from the path of the HCP, and \( L \) is the maximum depth of penetration of the delta rays from the surface of the detector, assuming that the incident particles are normal to the surface of the detector and that the HCP fluence is low. Figure 3.6 illustrates an incident HCP stopping inside of the detector, the symmetry of the problem and the adopted coordinate system.

The RDD function \( D(r, l) \) determines the mean absorbed energy from the incident HCP, \( E_{HCP} \):

\[ E_{HCP} = \Phi \int_0^{R_{Max}} \int_0^L D(r, l) \rho_m 2\pi r dr dl \]  

(3.17)
Figure 3.6: Illustration of HCP stopping inside of a detector to show the cylindrical symmetry of RDD. $R_{\text{Max}}$ is the maximum radial distance of the delta rays from the path of the HCP, and $L$ is the maximum depth of penetration of the delta rays from the surface of the detector.

Using eq. 3.16 and 3.17 we evaluate the efficiency to HCP as

$$
\eta_{\text{HCP}}(D) = \frac{\alpha^{-1} S_{\text{HCP}}}{E_{\text{HCP}}} = \frac{\int_0^{R_{\text{Max}}} \int_0^L \eta_\delta(D_0) f_\delta[D(r, l)] D(r, l) \rho_m 2\pi r dr dl}{\int_0^{R_{\text{Max}}} \int_0^L D(r, l) \rho_m 2\pi r dr dl} \tag{3.18}
$$

Dividing eq. 3.18 by eq. 3.13 we obtain the $\eta_{\text{HCP},\gamma}$ of HCP to the reference gamma radiation:

$$
\eta_{\text{HCP},\gamma}(D) = \frac{\eta_{\text{HCP}}(D)}{\eta_\gamma(D)} = \frac{\int_0^{R_{\text{Max}}} \int_0^L \eta_{\delta,\gamma}(D_0) f_\delta[D(r, l)] D(r, l) \rho_m 2\pi r dr dl}{f_\gamma(D) \int_0^{R_{\text{Max}}} \int_0^L D(r, l) \rho_m 2\pi r dr dl} \tag{3.19}
$$

For practical purposes the relative luminescence efficiency is defined in the “low dose” (linear) region of the reference gamma radiation field. In this case, $f_\gamma(D_0)$ simply equals unity and eq. 3.19 reduces to

$$
\eta_{\text{HCP},\gamma} = \frac{\int_0^{R_{\text{Max}}} \int_0^L \eta_{\delta,\gamma} f_\delta[D(r, l)] D(r, l) \rho_m 2\pi r dr dl}{\int_0^{R_{\text{Max}}} \int_0^L D(r, l) \rho_m 2\pi r dr dl} \tag{3.20}
$$

where

$$
\eta_{\delta,\gamma} = \eta'_\delta \frac{1}{W_{\text{HCP}}} \frac{1}{W_\gamma} \tag{3.21}
$$

We now make the TSM assumption: the ionization density is the only factor that in-
fluences the luminescence response of the detector. Thus, an infinitesimal volume of the detector exposed to radiation responds the same way as if the whole bulk of the detector was irradiated. Therefore, the luminescence signal from a detector exposed to HCP is a linear combination of luminescence signals from detectors exposed to a test radiation X that mimics as closely as possible the energy spectrum of delta rays produced by the primary particle. The test radiation X determines the luminescence response function, \( f_\delta[D(r, l)] \cong f_X[D(r, l)] \), and \( \eta_{HCP,\gamma} \) becomes

\[
\eta_{HCP,\gamma} = \frac{\int_0^{R_{\text{Max}}} \int_0^L \eta_{\delta,\gamma} f_X[D(r, l)]D(r, l)\rho_m 2\pi rdrdl}{\int_0^{R_{\text{Max}}} \int_0^L D(r, l)\rho_m 2\pi rdrdl}
\]  

(3.22)

Assuming that the energy of the incident HCP is large such that the change in the HCP LET is negligible when the HCP passes through the detector, as a first approximation, on average the delta rays deposit their energy uniformly through the whole depth of the detector, \( L \). Thus, the RDD can be approximated as \( D(r, l) \cong D(r) \) and the integrals in \( l \) on the numerator and denominator cancel out reducing eq. 3.22 to

\[
\eta_{HCP,\gamma} = \frac{\int_0^{R_{\text{Max}}} \eta_{\delta,\gamma} f_X[D(r)]D(r)\rho_m 2\pi rdr}{\int_0^{R_{\text{Max}}} D(r)\rho_m 2\pi rdr}
\]  

(3.23)

The above approximation is invalid for particles that stop inside of the detector, or for particles with energies such that the LET change inside of the detector is significant.

The integral in the denominator of eq. 3.23 is the total energy deposited by the HCP. Assuming that the energy transferred by the HCP is mainly through excitations and ionizations, producing delta rays, and that the delta rays do not have enough energy to escape the detector’s volume, the total energy deposited can be approximated as the \( L_\infty \) and the integral in the denominator is equal to the \( L_\infty \) of the incident HCP calculated in the detector’s material (index \( m \)), \( L_\infty^m \).

In eq. 3.23, the function \( f_X[D(r)] \) is determined experimentally through dose response measurements with the appropriate test radiation that mimics as closely as possible the
delta ray spectrum produced by the primary HCP. The factor $\eta_{\delta,\gamma}$ depends on the energy spectrum of secondary electrons and can be determined measuring the energy response to photon radiation. Chapter 8 presents discussions of the test radiation and determination of the energy dependent factor $\eta_{\delta,\gamma}$. Different models, simulation or experimental data provides the $D(r)$. Chapters 4 and 5 present different approaches in the determination of $D(r)$. 
CHAPTER 4

ANALYTICAL MODELING OF RADIAL DOSE DISTRIBUTION

A variety of models describes the RDD created by the passage of HCPs through matter. This chapter presents some of the models that are relevant to this work, including the models of Chatterjee and Schaefer (Chatterjee and Holley, 1993; Chatterjee and Schaefer, 1976), Butts and Katz (Butts and Katz, 1967; Hansen and Olsen, 1984; Chunxiang et al., 1985; Zhang et al., 1994), Waligórski et al. (Waligórski et al., 1986), Fageeha et al. (Fageeha et al., 1993), Kiefer and Straaten (Kiefer and Straaten, 1986), and Geiß et al. (Geiß et al., 1998; Krämer, 1995).

The main differences among the models are: the Chatterjee and Schaefer model simply assumes that the RDD is proportional to $r^{-2}$, where $r$ is the radial distance from the path of the incident HCP, whereas the Butts and Katz, Waligórski et al., Fageeha et al., and Kiefer and Straaten models use Rutherford’s single differential cross-section (SDCS) (Butts and Katz, 1967) to describe the number of secondary electrons produced by the HCP. Finally, the Geiß et al. model is a parameterization of Monte Carlo calculations of RDDs performed by Krämer (1995).

4.1 CHATTERJEE AND SCHAEFER MODEL

HCPs transfer energy mainly through collisions with electrons of the medium. Glancing collisions transferring small amounts of energy are much more frequent than close collisions transferring large amounts of energy. Thus, the Chatterjee and Schaefer model suggests an approximate equipartition of the total energy loss between glancing and close collisions (Chatterjee and Schaefer, 1976). The core is defined by them as the central re-
region of the track where glancing and close collisions prevail. In the core region the density
of energy deposition is very high. The core of the track is surrounded by a region called
penumbra where secondary electrons are the main event of energy deposition.

The equipartition of energy suggested by the Chatterjee and Schaefer model assigns
half of the total energy loss to glancing collisions and the other half to close collisions.
Glancing collisions are responsible for excitations and close collisions for ionizations. The
two types of collisions occur in the core region. On the other hand, only ionizations occur
in the penumbra region. Therefore, half or more of the energy loss by the incident particle
is in the core region.

\[
\begin{align*}
\text{Excitation} & \rightarrow \text{core} = \frac{L_m^m}{2} \\
\text{Ionization} & \rightarrow \text{core and penumbra} = \frac{L_m^m}{2}
\end{align*}
\]

where \( L_m^m \) is the unrestricted total linear energy transfer in the material of the detector
(index \( m \)) by the incident particle.

Considering a cylindrical geometry, the total energy loss due to excitation in an in-
finitesimal concentric cylindrical layer can be written as

\[
\frac{L_m^m}{2} = \rho_m \int_0^{r_c} D_{exc}(r) 2\pi r \, dr
\]

(4.1)

where \( D_{exc}(r) \) is the radial dose due to excitation, and \( \rho_m \) is the density of the medium.
The Chatterjee and Schaefer model assumes that in the core the radial dose is constant,
\( D_{exc}(r) = D_{exc}^c \). Thus, the integral of eq. 4.1 can be solved:

\[
D_{exc}^c = \frac{L_m^m / 2}{\pi r_c^2 \rho_m}
\]

(4.2)

The core and penumbra regions share the total energy loss due to ionizations. For a
charged particle traveling a distance $dz$

$$\frac{L_m}{2} = \rho_m \int_0^{r_c} D_{ion}(r) 2\pi r \ dr + \rho_m \int_{r_c}^{R_{\text{Max}}} D_{ion}(r) 2\pi r \ dr$$

(4.3)

where $D_{ion}(r)$ is the radial dose due to ionizations, and $r_c$ and $R_{\text{Max}}$ are the core and penumbra radius, respectively. Considering the radial dose constant in the core, $D_{ion}(r) = D_{ion}^c$. Chatterjee and Schaefer (1976) then assume that the radial dose in the penumbra due to ionization decreases with $r^2$, thus:

$$D_{ion}(r) = \begin{cases} 
D_{ion}^c, & r < r_c \\
\frac{r^2}{r_c^2}, & r_c < r < R_{\text{Max}} 
\end{cases}$$

(4.4)

So that eq. 4.3 gives:

$$\frac{L_m}{2\rho_m} = D_{ion}^c \int_0^{r_c} 2\pi r \ dr + D_{ion}^c \int_{r_c}^{R_{\text{Max}}} \frac{r^2}{r_c^2} 2\pi r \ dr$$

(4.5)

The radial dose due to ionization can be written as:

$$D_{ion}^c = \frac{\frac{L_m}{2\rho_m}}{\frac{r_c^2 \rho_m}{\frac{L_m}{2} \left(1 + 2 \ln \frac{R_{\text{Max}}}{r_c}\right)}}$$

(4.6)

Chatterjee and Schaefer (1976) determine the contribution of the radial dose in the core due to ionizations and excitations as:

$$D_c = D_{exc}^c + D_{ion}^c$$

(4.7)
Using eq. 4.2 and eq. 4.6 we obtain:

\[
D_c = \frac{L_m}{\pi r_c^2 \rho_m} + \frac{L_m}{\pi r_c^2 \rho_m} \left( \frac{1}{2} + 2 \ln \frac{R_{Max}}{r_c} \right) \tag{4.8}
\]

Chatterjee and Schaefer (1976) assign the events of energy deposition in the penumbra to ionizations only. So that

\[
D_p(r) = \frac{L_m}{\pi r^2 \rho_m} \left( \frac{1}{2} + 2 \ln \frac{R_{Max}}{r_c} \right) \tag{4.9}
\]

The next step is to present expressions for the radius of the core and penumbra regions. Chatterjee and Schaefer (1976) define the radius of the core as the region where the primary particle energy loss causes excitations of the surrounding atoms. The core radius is equal to the Bohr’s adiabatic limit region where electrons of the medium create an electric field directed against the motion of the primary particle Chatterjee and Holley (1993); Bohr (1948):

\[
r_c = \frac{v}{\Omega_p} \tag{4.10}
\]

where \(v\) is the velocity of the incident particle and \(\Omega_p\) is the plasma oscillation frequency, which is given by

\[
\Omega_p = \sqrt{\frac{4\pi N_e e^2}{m_e}} = c \sqrt{\frac{4\pi N_e r_e}{m_e}} \tag{4.11}
\]

where \(N_e\) is the density of electrons in the medium\(^1\), and \(e, m_e\) and \(r_e = 2.8179 \times 10^{-13}\) cm are the charge, mass and classical radius of the electron. The plasma oscillation frequency is the electrostatic oscillation frequency of the medium in response to a small charge displacement.

---

\(^1\)In water and Al\(_2\)O\(_3\) the density of electrons is \(3.34 \times 10^{23}\) electrons/cm\(^3\) and \(1.17 \times 10^{24}\) electrons/cm\(^3\), respectively.
Thus, the final expression for the core radius is:

\[ r_c = 5.314 \times 10^{12} \sqrt{N_e} \beta \text{ (nm)} \] (4.12)

where \( \beta = \frac{v}{c} \) is the relative speed of the incident particle with respect to the speed of light in vacuum, and \( N_e \) is the electron density of the material given in units of electrons/cm\(^3\).

Chatterjee and Holley (1993) define the penumbra radius by the empirical relation

\[ R_{Max} = \frac{3.85 \times 10^5}{\rho_m} \beta^{2.7} \text{ (nm)} \] (4.13)

where \( \beta = \frac{v}{c} \) is the relative speed of the primary particle with respect to the speed of light \( c \), and \( \rho_m \) is the density of the detector given in units of g/cm\(^{-3}\). Chatterjee and Schaefer (1976) determined the empirical relation given by eq. 4.13 by fitting range of electrons obtained through scattering theory and diffusion models (Chatterjee et al., 1973; Chatterjee and Schaefer, 1976).

Eq. 4.8 and eq. 4.9 together with eq. 4.12 and eq. 4.13 are the expressions to calculate the RDD around a HCP track according to the Chatterjee and Schaefer model. We summarize them as:

\[
D(r) = \begin{cases} 
\frac{L_m^m}{\pi r_c^2} + \frac{L_m^m}{\pi r_c^2} \left( 1 + 2 \ln \frac{R_{Max}}{r_c} \right), & r < r_c = 5.314 \times 10^{12} \sqrt{N_e} \beta \\
\frac{L_m^m}{\pi r^2} \left( 1 + 2 \ln \frac{R_{Max}}{r_c} \right), & r_c < r < R_{Max} = \frac{3.85 \times 10^5}{\rho_m} \beta^{2.7} 
\end{cases}
\] (4.14)

where \( L_m^m \), \( \rho_m \), and \( N_e \) must be in units of keV/\( \mu \)m, g/cm\(^{-3}\), and cm\(^{-3}\), respectively, so that \( D(r) \) is in Gy, and \( r, r_c, \) and \( R_{Max} \) in nm.

Figure 4.1 shows RDDs around the path of ions with different kinetic energies and atomic numbers, but with similar LET. The core radius depends on the density of electrons of the medium and on the velocity of the primary particle (eq. 4.12), and the penumbra
radius depends only on the velocity of the primary particle (eq. 4.13). Therefore, larger kinetic energies of the incident particles produce a larger core and penumbra radii. In the Chatterjee and Schaefer model, the core and penumbra radii are independent of the charge of the incident particle. The discontinuity in the interface between the core and penumbra regions was introduced for conducting the analytical process. Chatterjee and Schaefer (1976) state that there is no well defined border between the two regions.

![Chatterjee and Schaefer RDD in water](image)

**Figure 4.1:** Chatterjee and Schaefer RDD in water (eq. 4.14) around the path of oxygen (23 MeV/u) and iron (1000 MeV/u). The particles have approximately the same LET.

The problem with the Chatterjee and Schaefer model is that it is based on the equipartition of energy where half of the energy is deposited through excitation and the other half through ionization. However, recent publications indicate that only (5-10) % of the energy loss produces excitations for primary particles in the range from 0.5 MeV/u up to 100 MeV/u (IAEA, 1995).
4.2 BUTTS AND KATZ MODEL

Butts and Katz model uses Rutherford’s SDCS for production of secondary electrons (Mott, 1929; Bradt and Petters, 1948; ICRU, 1995). Rutherford’s secondary electron distribution formula gives the number of secondary electrons per unit of path length having energies in the interval from $w$ to $w + dw$, produced by an incident ion of effective charge $Z^*$ moving with speed $\beta c$

$$dn = \frac{2\pi N_e e^4 Z^{*2}}{m_e c^2 \beta^2 (w + I)^2} \frac{dw}{(w + I)^2} \quad (4.15)$$

where $m_e$ and $e$ are the electron mass and charge, $N_e$ is the density of electrons in the material, $I$ is the mean ionization potential of the material, $c$ is the speed of light and $\beta = v/c$ is the speed of the incident particle with respect to the speed of light. Considering water as the target material

$$\frac{2\pi N_e e^4}{m_e c^2} = 8.5 \times 10^{-3} \text{ keV} \mu \text{m} \quad (4.16)$$

Electrons with energy $w$ are ejected at an angle $\theta$ to the path of the incident moving ion where (Butts and Katz, 1967)

$$\cos^2 \theta = \frac{w}{W} \quad (4.17)$$

Since eq. 4.15 is proportional to $1/w^2$, the majority of secondary electrons have energies much less than maximum electron energy $W$ and therefore, have ejection angles approximately equal to $90^\circ$. Thus, to simplify the calculations Butts and Katz model assumes that all secondary electrons are ejected normally to the ion path (Butts and Katz, 1967).

Butts and Katz model uses the effective charge $Z^*$ expression given by Barkas (1963), which is a parameterization of experimental data:

$$Z^* = Z[1 - \exp(-125\beta Z^{-2/3})] \quad (4.18)$$

2The nuclear charge is shielded by orbital electrons and outer electrons will see an reduced nuclear charge as the effective charge $Z^*$ (Barkas, 1963).
where \( Z \) is the atomic number of the particle and \( \beta \) is the velocity of the particle relative to the speed of light in vacuum.

The Butts and Katz model range-energy relation for secondary electrons is a semi-empirical model obtained by fitting a power law relation to the experimental data (Butts and Katz, 1967; Chunxiang et al., 1985; Waligórski et al., 1986; Zhang et al., 1994). The range-energy relationship was fitted to the available experimental data of electron ranges in aluminum (Kobetich and Katz, 1968; Iskef et al., 1983; Kanter and Sternglass, 1962):

\[
t = kw^\alpha
\]

(4.19)

where \( t \) is the range of an electron of energy \( w \) and

\[
k = 6 \times 10^{-6} \text{ g cm}^{-2} \text{ keV}^{-\alpha}
\]

(4.20)

Two components characterizes the power law relation:

\[
w < 1 \text{ keV} \implies \alpha = 1.079
\]

\[
w > 1 \text{ keV} \implies \alpha = 1.667
\]

Differentiation of eq. 4.19 with respect to \( w \) leads

\[
\frac{dt}{t} = \alpha \frac{dw}{w}
\]

(4.21)

After penetrating a thickness \( r \) of material an electron of initial energy \( w \) and range \( t \) has a residual energy

\[
kw_r^\alpha = t - r
\]

(4.22)
Using eq. 4.19 we can write eq. 4.22 as

\[ w_r = w \left( 1 - \frac{r}{t} \right)^{\frac{1}{\alpha}} \] (4.23)

Differentiating eq. 4.23 with respect to \( r \), Butts and Katz model obtains the energy loss of electrons at a distance \( r \) from the path of the incident particle

\[ -\frac{dw_r}{dr} = \frac{w}{\alpha t} \left( 1 - \frac{r}{t} \right)^{\frac{1}{\alpha} - 1} \] (4.24)

An expression for the radial dose \( D(r) \) deposited in a cylindrical shell of thickness \( dr \) at radius \( r \) from the path of the incident ion can be written as (Waligórski et al., 1986)

\[ D(r) = \frac{1}{2\pi r dr \rho_m} \int_0^W \left( -\frac{dw_r}{dr} \right) dr \frac{dn}{dw} dw \] (4.25)

where \( 2\pi r dr \rho_m \) is the volume of the shell, \(-dw_r/dr\) is the energy loss, \( dn/dw \) is the number of electrons per path length with energy \( dw \),

\[ W = 2m_e c^2 \frac{\beta^2}{1 - \beta^2} \] (4.26)

is the maximum energy of a secondary electron in a head-on collision and

\[ kw_0^\alpha = r; \quad kI^\alpha = r_0; \quad kW^\alpha = R_{Max}; \] (4.27)

where \( I \) is the ionization potential of the material, \( R_{Max} \) is the maximum distance a delta ray can travel perpendicular to the path of the incident HCP, and \( r_0 \) is the distance perpendicular to the path of the incident HCP a delta ray of energy \( I \) can travel. Waligórski et al. (1986) considered the ionization potential \( I \) to be equal to 10 eV, so that \( r_0 = 0.426/\rho_m \) nm, where \( \rho_m \) is given in units of g/cm\(^{-3}\). Using eq. 4.15 and 4.23 the radial dose \( D(r) \)
can be written as

\[
D(r) = \frac{N_e e^4}{\alpha m_e c^2 \rho_m} \frac{Z^2}{\beta^2} \frac{1}{r} \int_{w_0}^{W} \frac{w}{t} \left(1 - \frac{r}{t}\right)^{1/\alpha - 1} \frac{dw}{(w + I)^2} \tag{4.28}
\]

To solve eq. 4.28 we set the ionization potential \( I = 0 \). Later on, the bound electron case is artificially included. Thus, taking \( I = 0 \) and using equation 4.21 we get

\[
D(r) = \frac{N_e e^4}{\alpha^2 m_e c^2 \rho_m} \frac{Z^2}{\beta^2} \frac{1}{r} \int_{r}^{R_{Max}} \left(1 - \frac{r}{t}\right)^{1/\alpha - 1} \frac{dt}{t^2} \tag{4.29}
\]

Substituting

\[
y = \frac{r}{t} \quad \text{and} \quad \frac{dt}{t^2} = -\frac{dy}{r}; \tag{4.30}
\]

\[
D(r) = -\frac{N_e e^4}{\alpha^2 m_e c^2 \rho_m} \frac{Z^2}{\beta^2} \frac{1}{r} \int_{1}^{r/R_{Max}} \left(1 - y\right)^{1/\alpha - 1} \frac{dy}{r} \tag{4.31}
\]

The transition from the free \((I = 0, r_0 = 0)\) to the bound \((r_0 = kI^\alpha)\) electron case is made by replacing \( r \) and \( R_{Max} \) within the final bracket by \( r + r_0 \) and \( R_{Max} + r_0 \), respectively. So that

\[
D(r) = \frac{N_e e^4}{m_e c^2 \rho_m} \frac{Z^2}{\alpha \beta^2} \frac{1}{r} \left[\left(1 - \frac{r + r_0}{R_{Max} + r_0}\right)^{1/\alpha}\right] \tag{4.32}
\]

If \( \rho_m \) and \( N_e \) are given in \( \text{g/cm}^3 \) and \( \text{cm}^3 \), respectively, \( D(r) \) is given in Gy and \( r \), \( r_0 \), and \( R_{Max} \) in nm, and eq. 4.32 becomes

\[
D(r) = 6.50 \times 10^{-22} \frac{N_e}{\rho_m} \frac{Z^2}{\alpha \beta^2} \frac{1}{r} \left[\left(1 - \frac{r + r_0}{R_{Max} + r_0}\right)^{1/\alpha}\right], \quad r_0 < r < R_{Max} \tag{4.33}
\]
where

\[
\alpha = \begin{cases} 
1.079, & \text{for } r_0 = 0.426/\rho_m < r < 61.3/\rho_m \\
1.667, & \text{for } 61.3/\rho_m < r < R_{\text{Max}} = 6.24 \times 10^6 \left( \frac{\beta^2}{1-\beta^2} \right)^{1.667} 
\end{cases}
\]

Figure 4.2 shows the RDD in water around the path of ions with different kinetic energies and atomic numbers, but with similar LET.

**Butts and Katz**


tagged series

\begin{align*}
\text{O: 23 MeV/u, 150 keV/\mu m} \\
\text{Fe: 1000 MeV/u, 144 keV/\mu m}
\end{align*}

Figure 4.2: Butts and Katz RDD in water (eq. 4.33) around the path of oxygen (23 MeV/u) and iron (1000 MeV/u). The particles have approximately the same LET. The ionization potential used on the plots was \( I = 10 \text{ eV} \).

### 4.2.1 MODIFICATIONS OF BUTTS AND KATZ MODEL

Waligórski et al. (1986) and Fageeha et al. (1993) modified Butts and Katz expression (eq. 4.33) by an arbitrary function of the form:

\[
D_{\text{cor}}(r) = D(r)[1 + K(r)]
\]  
(4.34)
Katz model to fit the experimental and Monte Carlo data in the region of small radius and also to correct the prediction of LET when the distribution of dose is radially integrated. This section describes the Waligórski et al. and the Fageeha et al. corrections.

**WALIGÓRSKI ET AL. CORRECTION**

Waligórski et al. used the following function

\[ K(r) = A \left( \frac{r - B}{C} \right) \exp \left( - \frac{r - B}{C} \right) \]  
(4.35)

where \( r \) is in nanometers and

(a) for \( r > B = 0.1 \) nm, \( C = 1.5 \) nm + 5 nm \( \times \beta \) and

\[ A = 8 \times \beta^{1/3}, \quad \text{for } \beta < 0.03 \]

or

\[ A = 19 \times \beta^{1/3}, \quad \text{for } \beta > 0.03 \]

(b) for \( r < B = 0.1 \) nm

\[ K(r) = 0 \]

Figure 4.3 compares the RDD from Butts and Katz model with the RDD from Waligórski et al. model. The Waligórski et al. model presents a hump at small radial distances and are equal to the Butts and Katz model at larger radius. This hump is observed in the experimental data of radial dose distribution (Waligórski et al., 1986). Another important feature is that the Waligórski et al. model improves the prediction of incident particle \( L_{\infty}^{H_2O} \).

\[ L_{\infty} = \rho_m \int_{r_0}^{R_{Max}} D(r) 2\pi r dr \]  
(4.36)

Table 4.1 presents the comparison of \( L_{\infty}^{H_2O} \) between the results given by Energy vs.
LET vs. Range calculator version 1.24\(^3\) (Zajic) and different RDD models. Note that the
\(L_\infty^{H_2O}\) predictions of Butts and Katz model is around 60\% below the correct value. The
Waligórski \textit{et al.} model improves the difference for \(L_\infty^{H_2O}\) around 15\% below the correct
value.

![Graph showing RDD in water around the path of oxygen (23 MeV/u). The full line is the Butts and
Katz model, dotted line is the Waligórski \textit{et al.} model and dashed line is the Fageeha \textit{et al.} model.]

\[ K(r) = A\beta^B (r - 0.1) \exp \left( -\frac{r}{C} \right) \]  

\(^3\)The program provided by Brookhaven National Laboratory calculates \(L_\infty\) and range for different mate-
rials, particles and energies.
Table 4.1: $L_{\infty}^{H_2O}$ determined using the Brookhaven National Laboratory (BNL) Energy vs. LET vs. Range calculator version 1.24 program and different RDD models.

<table>
<thead>
<tr>
<th>$Z$</th>
<th>Energy (MeV/u)</th>
<th>BNL</th>
<th>Butts and Katz</th>
<th>Waligórska et al.</th>
<th>Fageeha et al.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>230</td>
<td>0.41</td>
<td>0.15</td>
<td>0.36</td>
<td>0.45</td>
</tr>
<tr>
<td>1</td>
<td>70</td>
<td>0.96</td>
<td>0.31</td>
<td>0.78</td>
<td>1.06</td>
</tr>
<tr>
<td>2</td>
<td>150</td>
<td>2.18</td>
<td>0.75</td>
<td>1.85</td>
<td>2.40</td>
</tr>
<tr>
<td>6</td>
<td>400</td>
<td>10.96</td>
<td>3.96</td>
<td>9.65</td>
<td>11.9</td>
</tr>
<tr>
<td>6</td>
<td>290</td>
<td>12.97</td>
<td>4.62</td>
<td>11.3</td>
<td>14.1</td>
</tr>
<tr>
<td>8</td>
<td>400</td>
<td>19.48</td>
<td>7.03</td>
<td>17.2</td>
<td>21.1</td>
</tr>
<tr>
<td>10</td>
<td>400</td>
<td>30.44</td>
<td>11.0</td>
<td>26.8</td>
<td>32.9</td>
</tr>
<tr>
<td>26</td>
<td>500</td>
<td>186.3</td>
<td>67.7</td>
<td>164</td>
<td>200</td>
</tr>
<tr>
<td>54</td>
<td>290</td>
<td>1047</td>
<td>371</td>
<td>909</td>
<td>1135</td>
</tr>
</tbody>
</table>

where $r$ is in nanometers, $B = 0.215$, $C = 3.127 - 0.434\beta$, and

$$A = \begin{cases} 0, & \beta < 0.0081 \\ 112\beta - 0.899, & 0.0081 < \beta < 0.091 \\ 0.674\beta + 9.21, & \beta > 0.091 \end{cases}$$

Figure 4.3 compares Butts and Katz, Waligórska et al. and Fageeha et al. models. Fageeha et al. model presents the same hump at small radius observed in the Waligórska et al. model, and reduces to the Butts and Katz model at larger radius. The Fageeha et al. model improves the predictions of $L_{\infty}^{H_2O}$ to around 6% above the correct value (Table 4.1).

Although the Butts and Katz model agrees with the experimental data in the intermediate region of radial distances, the limitations are:

1. only energy deposition by secondary electrons is considered
2. energy deposition by excitations is not considered
3. the model agrees with $L_{\infty}^{H_2O}$ only after artificial correction using arbitrary functions
4. the model uses empirical data to obtain the range-energy relationship for electrons in aluminum
5. the fitted range-energy relation deviates from experimental data for high energy electrons, causing a wrong prediction for primary particles with total kinetic energy higher than approximately 300 MeV/u where the maximum secondary electron energy is around 800 keV

6. the model assumes that all delta rays are ejected normal to the ion’s path. This approximation underestimates the dose around the center of the track

7. the Rutherford’s SDCS for production of secondary electrons underestimates the experimental values. ICRU report 55 (ICRU, 1995) and chapter 5 discuss this issue.

### 4.3 KIEFER AND STRAATEN MODEL

Kiefer and Straaten model (Kiefer and Straaten, 1986) is based on the same assumptions made by Butts and Katz (1967):

1. heavy-ion produces secondary electrons in the exposed medium according to classical collision dynamics

2. the energy distribution of secondary electrons is proportional to the inverse of their initial energy

3. the range of the secondary electrons relates to their kinetic energy by a power law and the secondary electrons trajectories are straight lines

The angle between the direction of the primary HCP and secondary electron, $\theta$, is given by (Kiefer and Straaten, 1986)

$$
\sin^2 \theta = \frac{1 - w_0/w_{\text{max}}}{1 - w_0/2m_e c^2} \quad (4.38)
$$
Figure 4.4: Illustration of angular distributions and ranges of secondary electrons produced by HCPs (adapted from (Kiefer and Straaten, 1986)).
where \( w_0 \) is the starting energy of the secondary electron and \( w_{\text{max}} \) is the maximum value the starting energy \( w_0 \) can take. For non-relativistic cases \( w_{\text{max}} \) is:

\[
w_{\text{max}} = \frac{4AE(1 + E/2Mc^2)}{(1 + A)^2 + 2AE/Mc^2}
\]

(4.39)

where \( A = m_e/M \), \( E \) is kinetic energy of the primary particle, and \( m_e \) and \( M \) are the electron and HCP masses, respectively. For the non-relativistic case \( E << Mc^2 \) and since \( M >> m_e \), eq. 4.39 can be approximated as

\[
w_{\text{max}} = \frac{4m_e}{M} E
\]

(4.40)

Kiefer and Straaten (1986) determine the relationship between the range \( r \) of the secondary electrons and energy by fitting range-energy data for electrons in water from ICRU report 16 (ICRU, 1970) through:

\[
\rho_m r = kw^\alpha
\]

(4.41)

where \( \rho_m \) is the density of the medium in g/cm\(^3\), \( k = 5.26 \times 10^{-6} \) g/cm\(^2\) keV\(^{-\alpha}\) and \( \alpha = 1.70 \), so that \( r \) is given in nanometers. Kiefer and Straaten (1986) recommend using the \( k \) and \( \alpha \) values for electron energies in the interval from 200 eV up to 100 keV (Kiefer and Straaten, 1986).

The perpendicular distance from the center of the HCP path, \( x_0 \), of a secondary electron of starting energy \( w_0 \) is given by (Figure 4.4)

\[
x_0 = r \sin \theta
\]

(4.42)

Using eq. 4.38 and eq. 4.41:

\[
x_0^2 = k^2w_0^{2\alpha} \frac{1 - w_0/w_{\text{max}}}{1 - w_0/2m_ec^2}
\]

(4.43)
Differentiation of eq. 4.43 with respect to $w_0$ determines the penumbra radius $x_p$, the maximum perpendicular distance that an electron can travel from the path of the primary HCP. Kiefer and Straaten (1986) showed that the difference between $x_p$ calculated non-relativistically (i.e., $w_{max} << 2m_e c^2$) and relativistically for particles with energies up to 1000 MeV/u is only about 5%. Thus, Kiefer and Straaten (1986) considered the non-relativistic case and obtained:

$$x_p = k \left( \frac{2\alpha}{2\alpha + 1} \right)^{\alpha} \left( \frac{1}{2\alpha + 1} \right)^{\frac{1}{2}} w_{max}^\alpha$$

(4.44)

where the general numeric expression is

$$x_p = \frac{6.16 \times 10^1}{\rho_m} E^{1.7}$$

(4.45)

where $x_p$ is given in nm, providing $E$ and $\rho_m$ are in MeV/u and g/cm$^3$, respectively.

Using geometrical considerations Kiefer and Straaten (1986) determine the residual energy at a radial distance $x$ from the path of the primary particle (Figure 4.5):

$$\sin \theta = \frac{x_0 - x}{r'}$$

(4.46)

Using the range-energy relationship (eq. 4.41)

$$\frac{k w^\alpha}{\rho_m} \sin \theta = x_0 \left( 1 - \frac{x}{x_0} \right)$$

(4.47)

where $w$ is the residual energy of an secondary electron at distance $x$ which has a range $r'$.

$$w^\alpha = \frac{\rho_m x_0}{k} \left( 1 - \frac{x}{x_0} \right)$$

(4.48)
where \( r \) is the range of a secondary electron with initial energy \( w_0 \) (eq. 4.41). Finally, Kiefer and Straaten model obtains:

\[
w(x, w_0) = w_0 \left( 1 - \frac{x}{x_0} \right)^{\frac{1}{\alpha}}
\]  

(4.49)

The total energy \( w(x) \) deposited between \( x \) and \( x_p \) is determined integrating over the contributions of all electrons that have radial ranges \( x_0 \) larger than \( x \)

\[
w(x) = \int_{w_0_1}^{w_0_2} w(x, w_0) f(w_0) \, dw_0
\]  

(4.50)

where \( f(w_0) \, dw_0 \) is the distribution of secondary electron starting energies, assumed to have the form given by Butts and Katz (1967), which is the Rutherford’s formula for production of secondary electrons as previously discussed:

\[
f(w_0) \, dw_0 = \frac{2\pi N_e e^4 Z^*^2}{m_e c^2 \beta^2 w_0^2} \frac{1}{dw_0}
\]  

(4.51)

\( N_e \) is density of electron in the medium, \( e \) is the electron charge, \( m_e c^2 \) is the electron rest energy, \( Z^* \) is the effective charge of the primary particle (eq. 4.18), and \( \beta = v/c \) is the
speed of the primary particle relative to the speed of light in vacuum. Therefore,

\[ w(x) = \frac{2\pi N_e e^4 Z^2}{m_e c^2 \beta^2} \int_{w_0_2}^{w_0_1} \frac{1}{w_0} \left( 1 - \frac{x}{x_0} \right)^{\frac{1}{\alpha}} dw_0 \]  

(4.52)

Differentiating eq. 4.52 with respect to \( x \):

\[ -\frac{dw(x)}{dx} = \frac{2\pi N_e e^4 Z^2}{m_e c^2 \beta^2} \int_{w_0_2}^{w_0_1} \frac{1}{\alpha w_0 x_0} \left( 1 - \frac{x}{x_0} \right)^{\frac{1}{\alpha}-1} dw_0 \]  

(4.53)

The limits \( w_0_1 \) and \( w_0_2 \) are determined numerically as the roots of eq. 4.43 for \( x_0 = x \). Therefore, the integration of eq. 4.53 can only be performed numerically.

The dose as function of radial distance is given by

\[ D(x) = \frac{1}{2\pi \rho_m x} \frac{dw(x)}{dx} \]  

(4.54)

where \( \rho_m \) is the density of the medium, and \( x \) is the radial distance from the path of the primary HCP.

Results of numerical calculations showed that the RDD follows \( 1/x^2 \) dependence over many orders of magnitude. Thus, Kiefer and Straaten (1986) suggest that the functional dependence simply is

\[ D(r) = 3.82 \times 10^{-22} \frac{N_e Z^2}{\rho_m \beta^2} \frac{1}{r^2}, \text{ for } 0.1 \text{ nm} < r < x_p = R_{Max} = \frac{6.16 \times 10^1 E^{1.7}}{\rho_m} \]  

(4.55)

where we changed the notation \( x \) to \( r \), and \( D(r) \) is in Gy and \( r \) in nm, providing the input parameters are in the following units: \( \rho_m \) in g/cm\(^3\), \( N_e \) in cm\(^{-3}\), and \( E \) in MeV/u.

Figure 4.6 shows the RDD in water around the path of ions with different kinetic energies and atomic numbers, but with similar LET. The differences between the two RDDs are in the maximum range of secondary electrons and in the magnitudes of the dose – the doses for the O 23 MeV/u beam are higher than the doses for the Fe 1000 MeV/u beam.
The Kiefer and Straaten model is based on the Rutherford’s SDCS for production of delta rays as in the Butts and Katz model. As discussed before, the Rutherford’s formula considers only the energy loss by ionizations. The energy loss through excitations are not treated by the formalism. This influences the predictions of stopping powers. Other points that are not discussed by Kiefer and Straaten (1986) are the minimum radius of the track and how the deposited energy is shared between ionizations and excitations.

## 4.4 GEIß ET AL. MODEL

The Geiß et al. model (Geiß et al., 1998) is a parameterization of track structure calculations performed by Krämer (1995). Geiß et al. (1998), as did Chatterjee and Schaefer (1976), present both core and penumbra regions. The Monte Carlo calculations were pa-
rameterized as:

\[
D(r) = \begin{cases} 
  k, & r < r_c = 0.1 \text{ nm} \\
  k \left( \frac{r_c}{r} \right)^2, & r_c < r < R_{\text{Max}} 
\end{cases}
\]  (4.56)

where \( r_c \) is the core radius, \( R_{\text{Max}} \) is the maximum distance of delta rays, and \( k \) is a constant determined through the normalization of the RDD to the total energy loss per path length

\[
2\pi \int_0^{R_{\text{Max}}} D(r) r \, dr = \frac{1}{\rho} \frac{dE}{dx}
\]  (4.57)

The determination of \( R_{\text{Max}} \) is based on Monte Carlo calculations and is parameterized as:

\[
\rho_m R_{\text{Max}} = 4 \times 10^{-5} W^{\frac{1}{2}}
\]  (4.58)

where \( \rho_m \) is the density of the material, and \( W \) is the maximum energy of the delta ray given by eq. 4.26.

A final expression for Geiß et al. model is given by

\[
D(r) = \frac{1.602 \times 10^5}{\rho_m} \begin{cases} 
  \frac{L_{\infty}^m}{\pi r_c^2 \left( 1 + 2 \ln \frac{R_{\text{Max}}}{r_c} \right)}, & r < r_c = 0.1 \text{ nm} \\
  \frac{L_{\infty}^m}{\pi r^2 \left( 1 + 2 \ln \frac{R_{\text{Max}}}{r_c} \right)}, & r_c < r < R_{\text{Max}} = 1.31 \times 10^7 \rho_m \left( \frac{\beta^2}{1 - \beta^2} \right)^{\frac{3}{2}}
\end{cases}
\]  (4.59)

where \( \rho_m \) and \( L_{\infty}^m \) are in g/cm\(^{-3}\) and keV/\(\mu\)m, respectively, so that \( D(r) \) is in Gy, and \( r \) and \( R_{\text{Max}} \) in nm.

Figure 4.7 shows the RDD in water around the path of ions with different kinetic energies and atomic numbers, but with similar LET. The differences between the two RDDs are in the maximum range of secondary electrons and in the magnitudes of the dose – the doses for the O 23 MeV/u beam are higher compared to the doses for the Fe 1000 MeV/u beam.

Geiß et al. model is a simplified parameterization of Monte Carlo RDD calculations.
Figure 4.7: Geiß et al. RDD in water (eq. 4.56) around the path of oxygen (23 MeV/u) and iron (1000 MeV/u). The particles have approximately the same LET.

The size of the core is assumed to be constant and is independent on particle type and energy. Geiß et al. model arbitrarily chooses the core size equal to 0.1 nm.

4.5 SUMMARY OF ANALYTICAL MODELS OF RADIAL DOSE DISTRIBUTION

A common trend in the analytical models of RDD presented in this chapter is the approximated proportionality to $r^{-2}$ in the region of intermediate radial distances from the path of the incident particle. For intermediate radial distances all the models agree with each other (Figure 4.8), and with the experimental data (Wingate and Baum, 1976).

On the other hand, for small radial distances of about a few nanometers the RDDs drastically differ from model to model (Figure 4.8). Lack of RDD data in such small distances makes impossible the verification of the model that best describes the data.

Another difference presented among the models is in the maximum radial distance a
secondary electron can travel from the path of the incident particle \( R_{\text{Max}} \). For the same type of particle and energy, Chatterjee and Schaefer model gives the lowest \( R_{\text{Max}} \) and Geiß \textit{et al.} model the largest \( R_{\text{Max}} \) (Figure 4.8).

Table 4.2 shows a summary of the main features of each model presented in this chapter. The Butts and Katz, Waligórski \textit{et al.}, Fageeha \textit{et al.}, and Kiefer and Straaten models assume Rutherford’s SDCS for production of secondary electrons to derive the RDD formulas. The Chatterjee and Schaefer and Geiß \textit{et al.} models assume the existence of the core region, where the RDD is constant; and the penumbra region, where the RDD is proportional to \( r^{-2} \). In the Chatterjee and Schaefer model the core radius \( r_c \) is proportional to the speed of the incident particle in respect to the speed of light \( (\beta = v/c) \). On the other hand, with the Geiß \textit{et al.} model the core radius is constant and equal to 0.1 nm for all types of particles and energies.

Chatterjee and Schaefer, Butts and Katz, Waligórski \textit{et al.}, Fageeha \textit{et al.}, and Kiefer
Table 4.2: Summary of the main parameters of different RDD models. $r_c$ is the radius of the core region and $R_{Max}$ is the maximum radial distance of a secondary electron. SDCS stands for single differential cross-section and $\beta = v/c$ is the speed of the incident particle with respect to the speed of light in vacuum.

<table>
<thead>
<tr>
<th>Model</th>
<th>Assumption</th>
<th>$r_c$</th>
<th>$R_{Max}$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chatterjee and Schaefer</td>
<td>$D(r) \propto \begin{cases} k, &amp; r \leq r_c \ r^{-2}, &amp; r_c &lt; r &lt; r_p \end{cases}$</td>
<td>$\propto \beta$</td>
<td>$\propto \beta^{2.7}$</td>
</tr>
<tr>
<td>Butts and Katz</td>
<td>Rutherford’s SDCS</td>
<td>–</td>
<td>$\propto (\frac{\beta^2}{1-\beta^2})^{1.667}$</td>
</tr>
<tr>
<td>Waligórski et al.</td>
<td>Rutherford’s SDCS</td>
<td>–</td>
<td>$\propto (\frac{\beta^2}{1-\beta^2})^{1.667}$</td>
</tr>
<tr>
<td>Fageeha et al.</td>
<td>Rutherford’s SDCS</td>
<td>–</td>
<td>$\propto (\frac{\beta^2}{1-\beta^2})^{1.667}$</td>
</tr>
<tr>
<td>Kiefer and Straaten</td>
<td>Rutherford’s SDCS</td>
<td>–</td>
<td>$\propto (\frac{1}{\sqrt{1-\beta^2}} - 1)^{1.7}$</td>
</tr>
<tr>
<td>Geiß et al.</td>
<td>$D(r) \propto \begin{cases} k, &amp; r \leq r_c \ r^{-2}, &amp; r_c &lt; r &lt; r_p \end{cases}$</td>
<td>0.1 nm</td>
<td>$\propto (\frac{\beta^2}{1-\beta^2})^{2/2}$</td>
</tr>
</tbody>
</table>

and Straaten models use empirical relations to calculate the maximum radial distance $R_{Max}$ a secondary electron can travel from the path of the incident particle. On the other hand, Geiß et al. model uses parameterization of Monte Carlo calculations. Table 4.2 shows the dependence of $R_{Max}$ with respect to $\beta = v/c$ for the models presented in this chapter.

It is important to mention that the RDD models presented in the previous sections are only a small sample of the available models in the literature. We choose to present Chatterjee and Schaefer, Butts and Katz, Waligórski et al., Fageeha et al., Kiefer and Straaten, and Geiß et al. models mainly because these models are common in the literature related to luminescence detectors, their expressions are compact and simple, and they agree with available experimental data.
CHAPTER 5

MONTE CARLO MODELING OF RADIAL DOSE DISTRIBUTION

Monte Carlo (MC) is a numerical stochastic\(^1\) method used to find solutions of mathematical or physical problems. Specifically, for ionizing radiation interacting with matter, the method assumes that all probabilities (cross-sections) for elementary events in the life history of a particle are known. The MC method consists in following the primary particle and its secondaries throughout their life history. The elementary probabilities are used in each stage of the life history to determine the consecutive “state” of the particles until their energy is totally dissipated (Cashwell and Everett, 1959).

Among the multipurpose radiation MC codes, the most well known ones include GEANT4 (Agostinelli et al., 2003), FLUKA (Fassò et al., 2003, 2005), and MCNP/MCNPX (Boggs et al., 2005). This work uses GEANT4 version 8.1. We choose GEANT4 mainly because of its flexibility for experimental designing and the easy access to its physics documentation (Geant4-Collaboration, 2007b).

The interaction cross-sections with the medium dictate the stages of the life history of a particle interacting with matter. Thus, MC requires cross-section data and adequate physics models. This chapter presents GEANT4’s relevant cross-sections and physics models used to determine the RDDs. Also, the results of the RDDs obtained using GEANT4 are presented and compared with the analytical models.

\(^1\)Stochastic quantities are quantities which are subjected to random fluctuations.
5.1 SINGLE DIFFERENTIAL CROSS-SECTION FOR PRODUCTION OF SECONDARY ELECTRONS USED BY GEANT4

GEANT4 uses Bhabha (Bhabha, 1938), Massey and Corben (Rossi, 1952), and Oppenheimer et al. (Oppenheimer et al., 1940) single differential cross-sections (SDCS) for production of secondary electrons with energy in the interval \( T \) and \( T + dT \) by hadrons (Geant4-Collaboration, 2007b):

\[
\frac{d\sigma}{dT} = K Z \frac{Z^* \beta^2 T^2}{\beta^2 T^2} \left[ 1 - \beta^2 \frac{T}{T_{\text{max}}} \right]
\]

for spin 0

\[
\frac{d\sigma}{dT} = K Z \frac{Z^* \beta^2 T^2}{\beta^2 T^2} \left[ 1 - \beta^2 \frac{T}{T_{\text{max}}} + \frac{T^2}{2E^2} \right]
\]

for spin 1/2

\[
\frac{d\sigma}{dT} = K Z \frac{Z^* \beta^2 T^2}{\beta^2 T^2} \left[ \left( 1 - \beta^2 \frac{T}{T_{\text{max}}} \right) \left( 1 + \frac{T}{3Q_c} \right) + \frac{T^2}{3E^2} \left( 1 + \frac{T}{2Q_c} \right) \right]
\]

for spin 1

\( T_{\text{max}} \), the maximum energy transferable to free electrons, is calculated using classical collision theory for a head-on collision and is given by (Geant4-Collaboration, 2007b)

\[
T_{\text{max}} = \frac{2m_e c^2 (\gamma^2 - 1)}{1 + 2\gamma (m_e/M) + (m_e/M)^2}
\]

(5.2)

where \( \gamma = (1 - \beta^2)^{-\frac{1}{2}} \) is the relativistic factor. Eq. 5.2 does not consider effects of a mechanism known as Fermi-shuttle acceleration, which produces secondary electrons with energies higher than those obtained from two-body collision theory (Ohsawa et al., 2005b).

Note that when \( T \) is very small compared with the maximum transferable energy \( T_{\text{max}} \),
and with the factor $Q_c$, eq. 5.1 reduces to the classical expression known as the Rutherford’s formula:

$$\frac{d\sigma}{dT} = KZ \frac{Z^*^2}{\beta^2 T^2}$$

(5.3)

Thus, for small secondary electron energy compared to the energy of the incident particle, the SDCSs of different kinds of particles become identical and depend only on the energy $T$ of the secondary electron, and on $\beta$ of the primary particle (Rossi, 1952).

Ohsawa et. al (Ohsawa et al., 2005a,b; Sato et al., 2005) built an apparatus that allows measurements of the energy and angular distribution of secondary electrons with energies as low as 7 eV and as high as 10 keV. Such a device was used to measure double differential cross-sections (DDCS) for production of secondary electrons by 6 MeV/u and 10 MeV/u He$^{+2}$ ions in water vapor. The author kindly provided his raw data, which we compare in Figure 5.1 with two SDCS models: (i) Rutherford’s SDCS (eq. 5.3); and (ii) semi-empirical model by Rudd (ICRU, 1995; Rudd et al., 1992). Rudd’s SDCS is only applicable for ten materials, including water vapor. Rudd et al. (1992) and ICRU report 55 (ICRU, 1995) present a detailed description of Rudd’s and Rutherford’s SDCSs. The SDCS experimental data present the oxygen KLL Auger peak at $\sim$ 500 eV. The large SDCS for high energy electrons is attributed a mechanism known as Fermi-shuttle acceleration (Ohsawa et al., 2005b).

Figure 5.1 shows that Rutherford’s SDCS underestimates the data. In fact, the disagreement between Rutherford’s SDCS and data emphasizes the limitations of Rutherford’s SDCS. Most of the multipurpose MC codes, including GEANT4, as well as Butts and Katz, Waligórski et al., Fageeha et al., and Kiefer and Straaten models of RDD, uses Rutherford’s SDCS. The disagreement can be quantitatively presented through the calculation of the primary particle energy loss to medium by ionization, which is simply the integral of the single differential cross-section. The data give values of 0.193 MeV cm$^2$/mg, and 0.112 MeV cm$^2$/mg for the 6 MeV/u, and 10 MeV/u He$^{+2}$ ions, respectively. Rutherford’s SDCS gives 0.132 MeV cm$^2$/mg and 0.080 MeV cm$^2$/mg, respectively. A disagreement of about
Figure 5.1: Comparison between data (Ohsawa et al., 2005b) and models of SDCS for production of secondary electrons by 6 MeV/u and 10 MeV/u He$^{+2}$ ions in water vapor. Both graphs present the oxygen KLL Auger peak at $\sim$ 500 eV. Dr. D. Ohsawa kindly provided the data.
30 % is verified between data and the Rutherford’s SDCS for the primary particle energy loss to medium by ionization. When comparing to the total energy loss by the HCP to the medium by ionization and excitations, the total stopping power, the disagreement between data and Rutherford’s model is about 20 %. Thus, calculations of RDDs using Rutherford’s SDCS underestimate the results. Unfortunately, no universal method is available that yields accurate cross-sections for production of secondary electrons by HCPs for all primary and secondary energies and all target materials. Furthermore, the published SDCS experimental data is only for ten different media and primary particle energies below 10 MeV/u (Rudd et al., 1992; ICRU, 1995). These restrictions leave us with no other choices when dealing with general problems.

5.2 RADIAL DOSE DISTRIBUTION OBTAINED WITH GEANT4

MC provides a flexible approach to simulate RDDs. Physical parameters such as detector geometry and physics models can be conveniently modified. This section presents the description of the MC geometry and physics models used throughout this work and the influence of various physical parameters on the RDDs.

5.2.1 MODEL DESCRIPTION

The pattern of energy deposition by HCP exhibits radial symmetry. Thus, the natural geometry to use is cylindrical. In this work we use a cylinder divided into many concentric shells spaced from each other in logarithmic scale. Figure 5.2 illustrates the geometry utilized throughout this dissertation. The blue line represents the incident HCP, red lines the delta rays and yellow dots a MC step.

The number of concentric shells, radius $r$ and thickness $z$ of the cylinder, and material are input parameters and therefore can be conveniently varied.

To obtain the RDD, first we determined the energy deposited in each shell. The energy deposit in each shell was divided by the mass of the respective shell, and then normalized to
the number of particles used in the simulation. The number of particles varied for particles with different LETs. For low LET we used 1000 particles, and for high LET we used 100 particles. Thus, the RDD plots presented in this work are the average dose in each shell produced by one particle. We considered the radial distance from the path of the incident particle equal to the distance from the center of the cylinder to the center of each shell.

5.2.2 ENERGY DEPOSITED BY ELECTROMAGNETIC INTERACTION OF THE INCIDENT PARTICLE AND SECONDARY ELECTRONS

The RDD analytical models consider only the deposition of energy by the incident particle, secondary electrons, and highest order electrons (see chapter 4). Secondary photons, target and projectile fragments and other particles such as pions are disregarded in the RDD analytical models used in this work. Thus, to compare the MC simulations with the analytical models, we consider only the energy deposited by the incident particle and secondary electrons.

We use the class\(^2\) G4hLowEnergyIonisation (Geant4-Collaboration, 2007b) to calculate the energy loss due to ionization and production of secondary electrons by the incident HCP, and the class G4LowEnergyIonisation (Geant4-Collaboration, 2007b) to calculate the

\(^2\)In object-oriented programming, classes are independent logical units which can be developed in parallel to each other when creating large software systems such as GEANT4 (Geant4-Collaboration, 2007a).
energy loss due to ionization and production of highest order electrons by the secondary electrons produced by the incident HCP (Geant4-Collaboration, 2007b). Section 5.1 describes the cross-section for production of secondary electrons by the incident HCP. For the energy loss by the incident HCP, we use a parameterization model based on ICRU report 49 (ICRU, 1993) data. The transport of electrons was described by the Evaluated Electron Data Library (EEDL). Throughout this work we use a threshold of 250 eV for production of secondary electrons. The GEANT4 Physics Reference Manual (Geant4-Collaboration, 2007b) provides details about the physics models and parameterizations used by the classes G4hLowEnergyIonisation and G4LowEnergyIonisation. Appendix B presents the code relevant to the physics models used for the RDD simulations.

5.2.3 EFFECTS OF VARIOUS PARAMETERS IN THE RADIAL DOSE DISTRIBUTION

This subsection investigates the role of various parameters in the RDD MC simulations, including the maximum step size, number of particles, number of shells, and size of detector.

The maximum step size defines the precision of the MC calculations. At the beginning of a MC step, the code calls all active physics processes. Each process returns a step length. The code chooses the minimum step length. If the minimum step length is larger than the maximum step size defined by the user, the code uses the latter as the size of the MC step. Therefore, the maximum step size influences the computation time and affects the precision of the calculations; a smaller value produces a smoother RDD (Figure 5.3), however, the computation time increases.

As previously discussed, the values of the radial dose obtained are average values of dose per particle. Thus, as expected, Figure 5.4 shows that the RDD remains the same if the number of particles in the simulation increases. However, as the number of particle increases, the computation time also increases.
Figure 5.3: Influence of maximum step size on the RDD simulations of He 144.2 MeV/u ions in Al₂O₃:C.

Figure 5.4: Influence of the number of particles on the RDD simulations of He 144.2 MeV/u ions in Al₂O₃:C.
Figure 5.5 shows RDDs when changing the thickness $z$ of the detector. Note that the RDDs present a hump and are drastically changed by varying $z$. The hump moves to larger radial distances by increasing $z$. This hump is also observed in the Waligórski et al. and Fageeha et al. models of RDD (Figure 4.3), as well as experimental data (Waligórski et al., 1986).

GEANT4 determines the angular dependence of the ejected secondary electrons using conservation of momentum and energy (Geant4-Collaboration, 2007b). In Figure 5.2, the illustration on the left side shows the angular dependence of secondary electrons produced by the incident HCP. Note that secondary electrons with large energies ejected with small angles from the path of the incident particle also contribute to the dose. Thus, we expect to observe an angular dependence in the radial dose as the thickness $z$ of the absorber increases. Therefore, we attribute the hump to the angular dependence of the ejected secondary electrons with small angles.

![Graph showing RDD simulations with different thicknesses](image)

Figure 5.5: Influence of the thickness $z$ of the detector on the RDD simulations of He 144.2 MeV/u ions in Al$_2$O$_3$:C.

For very small values of $z$, most of the secondary electrons that contribute to the dose
are ejected perpendicular to the trajectory of the incident particle and the RDD agrees with the Butts and Katz model (Figure 5.5).

We observed a disagreement between the MC simulation and Butts and Katz model for radial distances smaller than the radial distance where the hump is located. For small radius, the MC simulations deviate from the $D \propto r^{-2}$ dependence. Also, as $z$ increases, the radial dose for small radius decreases. We performed various tests with different geometries, maximum step sizes, and when studying different interactions (scattering, bremsstrahlung, and energy threshold for production of secondary electrons) to understand the disagreement in the small radius, but we were unable to explain this dependence. Also, independent simulations using the FLUKA MC code performed by another group showed the same behavior of decreasing radial doses for small radius with increasing $z$ values (Mark et al., 2007).

The dependence on the thickness $z$ is an important point since the shape of the RDD influences on the predictions of $\eta_{HCP,\gamma}$. Chapter 8 emphasizes this dependence.
CHAPTER 6

EXPERIMENTAL DETAILS

As part of this dissertation, we performed irradiations in accelerators to characterize the response of OSL and TL detectors. This chapter describes the experimental details including preparation and types of detectors, facilities, irradiations, and readout methods.

6.1 DETECTORS AND PREPARATION

To study the difference in the $\eta_{\text{HCP},\gamma}$ of different materials, we use three types of detectors: $\text{Al}_2\text{O}_3$:C single crystals, $\text{Al}_2\text{O}_3$:C Luxel™, and LiF: Mg,Ti. $\text{Al}_2\text{O}_3$:C single crystals were grown at Urals Polytechnic Institute (Russia) and have an approximate diameter of 5.0 mm and a thickness of 0.9 mm. Luxel™ detectors (Landauer Inc.) are thin strips with dimensions 2.0 cm × 1.7 cm × 0.3 mm containing powdered $\text{Al}_2\text{O}_3$:C. From each as-received Luxel™ strip we cut 16 square pieces ($\sim 3$ mm × 3 mm), or 5 punched circular pieces ($\sim 7$ mm diameter). LiF: Mg,Ti detectors (TLD-100, Harshaw Research Group™) are in the form of hot pressed chips with natural isotopic abundance of Li. Each TLD-100 chip has the dimensions 3.2 mm × 3.2 mm × 0.9 mm.

We used two types of detector packages for the irradiations: (i) detectors packed with black electrical tape to protect the optically stimulated luminescence detectors (OSLDs) from light, and mounted in polycarbonate (Lexan™) holders of dimensions 7.0 cm × 3.5 cm × 0.7 cm, or (ii) detectors simply packed with black electrical tape. For the detectors mounted in polycarbonate holders, the HCP beam traversed a polycarbonate thickness of 2.0 mm before reaching the detectors. Tests performed with both types of packaging showed that the holder has no influence on the results. For particles with small range, we
Table 6.1: Pre-irradiation treatments for the detectors used in this study: Luxel\textsuperscript{TM}, \( \text{Al}_2\text{O}_3\text{C} \) single crystals and TLD-100.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Readout</th>
<th>Thickness</th>
<th>Annealing/bleaching</th>
</tr>
</thead>
<tbody>
<tr>
<td>Luxel\textsuperscript{TM}</td>
<td>OSL</td>
<td>0.3 mm</td>
<td>Yellow light overnight</td>
</tr>
<tr>
<td>( \text{Al}_2\text{O}_3\text{C} )</td>
<td>OSL/TL</td>
<td>0.9 mm</td>
<td>900 °C/15 min</td>
</tr>
<tr>
<td>TLD-100</td>
<td>TL</td>
<td>0.9 mm</td>
<td>400 °C/1 h + 100 °C/2 h</td>
</tr>
</tbody>
</table>

used the packing with black electrical tape only.

To eliminate any background signal accumulated during storage of the detectors before irradiation, the detectors were bleached or annealed. Luxel\textsuperscript{TM} detectors were illuminated overnight with yellow light from a halogen lamp filtered by a yellow glass filter Kopp 3-69 (Bøtter-Jensen et al., 2003). \( \text{Al}_2\text{O}_3\text{C} \) single crystal detectors were annealed at 900 °C for 15 min (McKeever et al., 1995). TLD-100 detectors were annealed at 400 °C for 1 h following 100 °C for 2 h (McKeever et al., 1995). After bleaching or annealing, the detectors presented a background signal lower than the dark counts of the photomultiplier.

Table 6.1 shows the type of detectors, thickness and reset treatment procedures. After the reset treatments the Luxel\textsuperscript{TM} and \( \text{Al}_2\text{O}_3\text{C} \) single crystal were enclosed in black plastic or black electrical tape to avoid exposure to light.

### 6.2 HEAVY CHARGED PARTICLE IRRADIATIONS

We performed irradiations with 24 combinations of particles and energies at four different facilities: Heavy Ion Medical Accelerator in Chiba (HIMAC) at National Institute of Radiological Sciences (NIRS), Japan; NASA Space Radiation Laboratory (NSRL) at Brookhaven National Laboratory (BNL), USA; Loma Linda University Medical Center (LLUMC), USA; and Texas A & M University (TAMU), USA. Some of the irradiations were performed during the ICCHIBAN project (Inter-Comparison for Cosmic-rays with Heavy Ion Beams at NIRS), and as part of investigations carried out by other groups (courtesy of E. R. Benton, Eril Research Inc; and E. Semones and R. Gaza, Space Radiation
The HCPs used in this study covered atomic numbers from 1 (proton) to 54 (xenon), and energies from 14 MeV/u to 1000 MeV/u, corresponding to $L_{\infty}$ in water from 0.223 keV/µm to 1368 keV/µm, $L_{\infty}$ in LiF:Mg,Ti (density of 2.64 g/cm$^3$) from 0.474 keV/µm to 2899 keV/µm, and $L_{\infty}$ in Al$_2$O$_3$:C (density of 3.97 g/cm$^3$) from 0.734 keV/µm to 4462 keV/µm.

For most of the irradiations, the accelerator facility’s staff provided us measurements of the range of the HCP in water. The ranges were measured using material with thickness equivalent to that of a slab of water (water equivalent binary filters). We use the Energy vs. LET vs. Range calculator version 1.24 build by Vladimir Zajic at Brookhaven National Laboratory (Zajic) to calculate the $L_{\infty}$ values, and range in other materials (Al$_2$O$_3$:C and LiF:Mg,Ti).

Table 6.2 summarizes the beams and experiments, nominal and actual energies, $L_{\infty}$ and range in water, LiF:Mg,Ti and Al$_2$O$_3$:C for all the HCP irradiations we have performed so far.

The delivered doses to the detectors were determined at the facility with plastic scintillation counters and ion chambers calibrated against gamma rays from a $^{60}$Co to absorbed dose to water.

Throughout this work we use the nominal energy of the HCP to label the irradiations. For instance, a helium ion with nominal energy of 150 MeV/u and actual energy of 144.2 MeV/u is referred in the text as He 150 MeV/u. All the LET values presented here, however, are from the actual energy of the beams.

### 6.3 CALIBRATION OF A $^{90}$Sr/$^{90}$Y SOURCE AGAINST A $^{60}$Co SOURCE

In addition to the HCP irradiations, we also performed irradiations with a $^{90}$Sr/$^{90}$Y source for studies of dose response and calibration purposes. The $^{90}$Sr/$^{90}$Y beta source is build into the Risø TL/OSL-DA-15 reader (Bøtter-Jensen et al., 2000). The dose rate de-
Table 6.2: Beam characteristics of the HCP irradiations.

<table>
<thead>
<tr>
<th>Beam</th>
<th>Energy (MeV/u)</th>
<th>$L_{\infty}$ in H$_2$O (keV/µm)</th>
<th>Range in H$_2$O (cm)</th>
<th>$L_{\infty}$ in LiF:Mg,Ti (keV/µm)</th>
<th>Range in LiF:Mg,Ti (cm)</th>
<th>$L_{\infty}$ in Al$_2$O$_3$:C (keV/µm)</th>
<th>Range in Al$_2$O$_3$:C (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proton 1000 MeV</td>
<td>1000$^a$</td>
<td>0.223</td>
<td>327</td>
<td>0.474</td>
<td>154</td>
<td>0.734</td>
<td>99.4</td>
</tr>
<tr>
<td>H 230 MeV</td>
<td>230$^a$</td>
<td>0.413</td>
<td>33.1</td>
<td>0.875</td>
<td>15.7</td>
<td>1.35</td>
<td>10.2</td>
</tr>
<tr>
<td>H 70 MeV</td>
<td>70$^a$</td>
<td>0.960</td>
<td>4.09</td>
<td>2.02</td>
<td>1.95</td>
<td>3.10</td>
<td>1.28</td>
</tr>
<tr>
<td>H 40 MeV</td>
<td>40$^a$</td>
<td>1.50</td>
<td>1.49</td>
<td>3.14</td>
<td>0.714</td>
<td>4.79</td>
<td>0.470</td>
</tr>
<tr>
<td>H 30 MeV</td>
<td>30$^a$</td>
<td>1.90</td>
<td>0.888</td>
<td>3.95</td>
<td>0.426</td>
<td>6.02</td>
<td>0.281</td>
</tr>
<tr>
<td>He 150 MeV/u</td>
<td>144.2</td>
<td>2.24</td>
<td>14.7</td>
<td>4.75</td>
<td>6.95</td>
<td>7.31</td>
<td>4.54</td>
</tr>
<tr>
<td>H 24 MeV</td>
<td>24$^a$</td>
<td>2.27</td>
<td>0.593</td>
<td>4.73</td>
<td>0.285</td>
<td>7.19</td>
<td>0.189</td>
</tr>
<tr>
<td>H 20 MeV</td>
<td>20$^a$</td>
<td>2.64</td>
<td>0.427</td>
<td>5.48</td>
<td>0.206</td>
<td>8.31</td>
<td>0.136</td>
</tr>
<tr>
<td>H 17 MeV</td>
<td>17$^a$</td>
<td>3.01</td>
<td>0.319</td>
<td>6.24</td>
<td>0.154</td>
<td>9.45</td>
<td>0.102</td>
</tr>
<tr>
<td>H 14 MeV</td>
<td>14$^a$</td>
<td>3.52</td>
<td>0.225</td>
<td>7.29</td>
<td>0.109</td>
<td>11.02</td>
<td>0.072</td>
</tr>
<tr>
<td>C 400 MeV/u</td>
<td>386.9</td>
<td>11.14</td>
<td>25.9</td>
<td>23.71</td>
<td>12.2</td>
<td>36.52</td>
<td>7.93</td>
</tr>
<tr>
<td>C 290 MeV/u</td>
<td>277.2</td>
<td>13.30</td>
<td>15.0</td>
<td>28.22</td>
<td>7.07</td>
<td>43.51</td>
<td>4.60</td>
</tr>
<tr>
<td>O 1000 MeV/u</td>
<td>1000$^a$</td>
<td>14.24</td>
<td>80.9</td>
<td>30.33</td>
<td>38.1</td>
<td>46.97</td>
<td>24.6</td>
</tr>
<tr>
<td>O 400 MeV/u</td>
<td>385.5</td>
<td>19.84</td>
<td>19.2</td>
<td>42.11</td>
<td>9.10</td>
<td>65.03</td>
<td>5.91</td>
</tr>
<tr>
<td>C 135 MeV/u</td>
<td>111.2</td>
<td>24.41</td>
<td>3.08</td>
<td>51.62</td>
<td>1.46</td>
<td>79.28</td>
<td>0.956</td>
</tr>
<tr>
<td>Ne 400 MeV/u</td>
<td>371.9</td>
<td>31.55</td>
<td>14.6</td>
<td>66.98</td>
<td>6.87</td>
<td>103.4</td>
<td>4.46</td>
</tr>
<tr>
<td>Si 490 MeV/u</td>
<td>444.8</td>
<td>56.80</td>
<td>13.8</td>
<td>120.7</td>
<td>6.54</td>
<td>186.4</td>
<td>4.24</td>
</tr>
<tr>
<td>Ar 500 MeV/u</td>
<td>450.7</td>
<td>93.34</td>
<td>12.2</td>
<td>198.3</td>
<td>5.77</td>
<td>306.4</td>
<td>3.74</td>
</tr>
<tr>
<td>Ti 1000 MeV/u</td>
<td>977.6</td>
<td>108.2</td>
<td>31.1</td>
<td>230.4</td>
<td>14.7</td>
<td>356.9</td>
<td>9.48</td>
</tr>
<tr>
<td>Fe 1000 MeV/u</td>
<td>967.0</td>
<td>151.4</td>
<td>25.6</td>
<td>322.5</td>
<td>12.1</td>
<td>499.4</td>
<td>7.80</td>
</tr>
<tr>
<td>Fe 500 MeV/u</td>
<td>423.7</td>
<td>200.3</td>
<td>7.45</td>
<td>425.3</td>
<td>3.43</td>
<td>657.0</td>
<td>2.28</td>
</tr>
<tr>
<td>Fe 200 MeV/u</td>
<td>120.4</td>
<td>431.8</td>
<td>0.905</td>
<td>912.8</td>
<td>0.430</td>
<td>1403</td>
<td>0.281</td>
</tr>
<tr>
<td>Kr 400 MeV/u</td>
<td>313.1</td>
<td>447.2</td>
<td>6.38</td>
<td>948.9</td>
<td>1.70</td>
<td>1464</td>
<td>1.11</td>
</tr>
<tr>
<td>Xe 290 MeV/u</td>
<td>185.5</td>
<td>1368</td>
<td>11.0</td>
<td>2899</td>
<td>0.520</td>
<td>4462</td>
<td>0.339</td>
</tr>
</tbody>
</table>

$^a$Nominal energy of the beam.
Table 6.3: Dose rate of $^{90}$Sr/$^{90}$Y beta source calibrated against a $^{60}$Co source from NIST in absorbed dose rate to water for all the detectors and readout procedures used in this work.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Readout procedure</th>
<th>Filter</th>
<th>Emission band</th>
<th>Dose rate (mGy/s)</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Luxel$^\text{TM}$</td>
<td>OSL</td>
<td>U-340 + WG-360</td>
<td>F-center</td>
<td>95.0</td>
<td>August 28, 2005</td>
</tr>
<tr>
<td>Luxel$^\text{TM}$</td>
<td>OSL</td>
<td>U-340</td>
<td>F-center + UV</td>
<td>82.0</td>
<td>August 28, 2005</td>
</tr>
<tr>
<td>Al$_2$O$_3$:C</td>
<td>OSL</td>
<td>U-340</td>
<td>F-center + UV</td>
<td>52.4</td>
<td>April 18, 2006</td>
</tr>
<tr>
<td>Al$_2$O$_3$:C</td>
<td>TL</td>
<td>5-58</td>
<td>F-center</td>
<td>52.4</td>
<td>April 18, 2006</td>
</tr>
<tr>
<td>TLD-100</td>
<td>TL</td>
<td>BG-39</td>
<td>Peak 5</td>
<td>69.4</td>
<td>May 8, 2004</td>
</tr>
</tbody>
</table>

The dose rate was obtained through calibration of the source against a $^{60}$Co gamma source from National Institute of Standards and Technology (NIST), courtesy of Dr. C. Soares. An independent calibration was performed against the NIST standards for each combination of material (Luxel$^\text{TM}$, Al$_2$O$_3$:C single crystal, TLD-100), signal (OSL total area, TL peak height) and optical filter (Hoya U-340, Schott WG-360, Corning 5-58, Schott BG-39) (Table 6.3).

Luxel$^\text{TM}$ detectors give different dose rates when OSL is measured with different procedures. This difference is due to the luminescence from the UV emission band, which increases with time elapsed since irradiation (Yukihara and McKeever, 2006b).

Throughout this dissertation we report the absorbed doses as $^{60}$Co gamma rays absorbed doses to water, unless explicitly specified.

### 6.4 OPTICALLY STIMULATED LUMINESCENCE READOUTS

A Risø TL/OSL-DA-15 reader (Botter-Jensen et al., 2000) was used for continuous wave OSL readouts. The OSL readouts consisted of stimulation for 300 s of the detectors with green light from light emitting diodes (LEDs), with emission centered at 525 nm and power of approximately 10 mW/cm$^2$ at the detector’s surface.

For the OSL measurements we use two different sets of filter packages to: i) discriminate the stimulation light from the luminescence light; and ii) select appropriate detection windows to measure luminescence from the F-center and UV emission bands, or F-center
emission band only in Al$_2$O$_3$:C. One of the sets, labeled set 1, is composed of Hoya U-340 filters (transmission centered at 340 nm, FWHM = 80 nm) with a thickness of 7.5 mm (Figure 6.1a) and allows detection of both F-center and UV emission bands of Al$_2$O$_3$:C (Yukihara and McKeever, 2006b). The other filter package, labeled set 2, is composed of 2 mm thick long-pass Schott WG-360 (cutoff at 360 nm) and 7.5 mm thick Hoya U-340 filter (Figure 6.1a), allowing detection only of the main emission band of Al$_2$O$_3$:C (F-center centered at 420 nm).

Throughout this work we consider the OSL signal equal to the total area under the OSL curve. The background signal of the OSL curve was considered to be the average of the last ten points in the OSL curve. We subtracted the background signal for all the analysis (Figure 6.2). Table 6.4 summarizes the stimulation power and wavelength, type of filters and detection window and analysis of the OSL signal.

All the OSL data presented in this work are the average of three OSL measurements and the error bars are one standard deviation of the data.

### 6.5 THERMOLUMINESCENCE READOUTS

A Risø TL/OSL-DA-15 reader with a linear heating rate and in N$_2$ atmosphere was used for the TL readouts.

The TL from Al$_2$O$_3$:C single crystal detectors was measured with linear heating rate of 1 °C/s and a 4 mm thick Corning 5-58 filter (transmission centered at 410 nm, FWHM = 80 nm) to select the main emission band (F-center) of Al$_2$O$_3$:C at 420 nm (Figure 6.1b).

The TL from TLD-100 was measured with linear heating rates of 1 °C/s and 5 °C/s and 6 mm thick Schott BG-39 filter (transmission centered at 475 nm, FWHM = 250 nm) (Figure 6.1b).

We considered the TL signal from Al$_2$O$_3$:C single crystal detectors equal to the height of the TL peak (Figure 6.3a), and the TL signal from TLD-100 equal to the height of the main TL peak (peak 5) (Figure 6.3b).
Figure 6.1: Transmission of a) Hoya U-340 and Schott WG-360 filters used in the OSL readouts and b) Schott BG-39 and Corning 5-58 filters used in the TL readouts.
Figure 6.2: Typical OSL curve from Luxel™ detectors. We considered the OSL signal equal to the total area under the OSL curve subtracting the background signal.

Table 6.4 summarizes the parameters of the OSL and TL measurements.

All the TL data presented in this work are the average of three TL measurements and the error bars are one standard deviation of the data.

### 6.6 CALIBRATION METHOD

A calibration curve was determined for each type of detector using irradiations with known doses. The methodology uses a second irradiation with a fixed reference dose to account for the sensitivity of each detector. In Luxel™ detectors this method allows measurements of doses with uncertainties lower than 0.7% for a single measurement (Yukihara et al., 2005).

The calibration curve is constructed using the ratio $S/S_R$, where $S$ is the signal of the detector irradiated with a known dose $D$, and $S_R$ is the signal of the detector irradiated with a reference dose $D_R$. The calibration curve is fitted using a saturating exponential (Figure...
Figure 6.3: Typical TL curves of a) $\text{Al}_2\text{O}_3$:C single crystal, and b) TLD-100 detectors. We considered the TL signal from $\text{Al}_2\text{O}_3$:C single crystal and TLD-100 equal to the height of their dosimetric TL peaks.
Table 6.4: Summary of readout methods, and filter packages used for OSL and TL measurements.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Method</th>
<th>Heating rate</th>
<th>Stimulation</th>
<th>Detection (filters)</th>
<th>Signal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Luxel&lt;sup&gt;TM&lt;/sup&gt;</td>
<td>OSL</td>
<td>none</td>
<td>10 mW/cm&lt;sup&gt;2&lt;/sup&gt; at 525 nm (green LEDs)</td>
<td>Set 1: Hoya U-340 (centered at 340 nm, FWHM = 80 nm)</td>
<td>Area (integrated over 300 s or 600 s) (F-center and UV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Set 2: Schott WG-360 (long-pass 360 nm) and Hoya U-340</td>
<td>Area (integrated over 300 s or 600 s) (F-center and UV)</td>
</tr>
<tr>
<td>Al&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;::C</td>
<td>OSL</td>
<td>none</td>
<td>10 mW/cm&lt;sup&gt;2&lt;/sup&gt; at 525 nm (green LEDs)</td>
<td>Set 1: Hoya U-340 (centered at 340 nm, FWHM = 80 nm)</td>
<td>Area (integrated over 300 s or 600 s) (F-center and UV)</td>
</tr>
<tr>
<td>single crystal</td>
<td></td>
<td></td>
<td></td>
<td>Set 2: Schott BG-39 (centered at 410 nm, FWHM = 80 nm)</td>
<td>Peak height (F-center)</td>
</tr>
<tr>
<td>TLD-100</td>
<td>TL</td>
<td>1 °C/s</td>
<td>none</td>
<td>Schott BG-39 (centered at 475 nm, FWHM = 250 nm)</td>
<td>Peak height (peak 5)</td>
</tr>
</tbody>
</table>

6.4). To determine an unknown HCP dose, first we measure the OSL signal \( S \) using the same setup (type of detector, filters and equipment), and then we give the same reference dose \( D_R \) adopted in the calibration curve to determine \( S_R \). Next we calculate the ratio \( S/S_R \) and using the calibration curve we determine the dose \( D \) (Figure 6.4).

This calibration method considers that HCP, gamma, and beta radiations produce the same sensitivity changes in the detectors. Doses received during transportation and storage were carefully subtracted from the HCP doses delivered at the facilities through evaluation of control detector packages, transported and stored together with the irradiated detectors.
Figure 6.4: Example of calibration curve using the reference dose method. The full line is the fit to the three data points using a saturated exponential. The value of the fitting parameters are: $A = 7.54 \pm 1.8$, and $B = (4.02 \times 10^4 \pm 1.10 \times 10^4) \text{ Gy}^{-1}$.
CHAPTER 7

OPTICALLY STIMULATED LUMINESCENCE PROPERTIES OF $\text{Al}_2\text{O}_3$:C EXPOSED TO DIFFERENT IONIZATION DENSITIES

The OSL curves from $\text{Al}_2\text{O}_3$:C depend on the ionization density of the radiation. Therefore, characterization of the differences in the response of the detector to various ionization densities is important. This chapter presents OSL data from Luxel$^\text{TM}$ detectors exposed to a combination of 24 particles and energies. First, we present the dose response and analysis of the shape of the OSL curve for Luxel$^\text{TM}$ detectors irradiated with nine radiation qualities: gamma ray from a $^{60}\text{Co}$ source, beta ray from a $^{90}\text{Sr}^{90}\text{Y}$ source, H 1000 MeV, He 150 MeV/u, Ne 400 MeV/u, Si 490 MeV/u, Fe 1000 MeV/u, Fe 500 MeV/u and Fe 200 MeV/u. Then, we present $\eta_{HCP,\gamma}$ versus $L_\infty$ in water. Appendix A presents a complete table with TL and OSL $\eta_{HCP,\gamma}$ values for $\text{Al}_2\text{O}_3$:C single crystal and TLD-100 detectors.

7.1 DOSE RESPONSE

We irradiated Luxel$^\text{TM}$ detectors in the interval of absorbed dose from 1 mGy to 10 kGy with: beta particles from a $^{90}\text{Sr}^{90}\text{Y}$ source, exposed at Oklahoma State University (OSU) in the Risø TL/OSL-DA-15 reader; He 150 MeV/u, Ne 400 MeV/u, Si 490 MeV/u, Fe 500 MeV/u and Fe 200 MeV/u, exposed at HIMAC by OSU in 2006; and H 1000 MeV and Fe 1000 MeV/u, exposed at NSRL by Eril Research Inc. in 2006. Table 6.2 presents the parameters of the beams such as actual energy, and LET.

Dose response curves and luminescence response functions $f(D)$ were plotted to analyze the linearity of the detector to different radiation qualities. To study the role of the UV
emission band in the OSL of Luxel\textsuperscript{TM} detectors, the measurements were performed using different filters to measure either a combination of F-center and UV emission bands, or the F-center emission band alone.

### 7.1.1 BETA RAYS DOSE RESPONSE

Figures 7.1a and 7.1b present the dose response and luminescence response function when measuring F-center and UV emission bands simultaneously (Hoya U-340 filter), and Figures 7.1c and Figure 7.1d present the dose response and luminescence response function when measuring only the F-center emission band (Hoya U-340 and Schott WG-360 filters).

Figure 7.1: OSL dose response and luminescence response function of Luxel\textsuperscript{TM} detectors irradiated with beta rays from a $^{90}$Sr/$^{90}$Y source. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) represent arbitrary functions fitted to the data for better visualization.

Note that the dose response curve, and therefore, the luminescence response function of
Luxel\textsuperscript{TM} detectors depends drastically on the detection filter. The luminescence response function (eq. 3.10), which describes how the signal deviates from linearity, presents a maximum supralinearity equal to 1.8 at 85 Gy when F-center and UV emission bands are detected, and \(\sim 1.2\) at 45 Gy when only F-center emission band is detected. For both detection filters, the saturation starts to occur above approximately 100 Gy. These results agree with previous results (Yukihara and McKeever, 2006b; Edmund et al., 2007b).

Yukihara et al. (2004b) explained the supralinearity of the F-center emission band by a competing mechanism of filling of deep electron and hole traps and correlated changes in the concentration of recombination centers (\(F^\pm\)-centers) and OSL sensitivity. In the case of the \(\text{Al}_2\text{O}_3:\text{C}\) samples used in this study (Luxel\textsuperscript{TM}), the supralinearity is due to an unknown recombination center responsible for the UV emission band, whereas the OSL signal corresponding to F-center emission band presents a small supralinearity. In this case, the model proposed by Yukihara et al. (2004b) does not explain the supralinearity of the UV emission band, and the explanation requires a better understanding of the nature of the defects responsible for the UV emission band and their role in the OSL process.

### 7.1.2 HEAVY CHARGED PARTICLE DOSE RESPONSE

As in the study of the luminescence response to beta rays (see subsection 7.1.1), the dose response curves and luminescence response functions \(f(D)\) were plotted to analyze the linearity of the detector to different radiation qualities. The measurements were performed using different filters to select either a combination of the F-center and UV emission bands, or only the F-center emission band. Next we discuss the dose response and \(f(D)\) for seven different HCP beams (Figure 7.2 through Figure 7.8).

For H 1000 MeV irradiation a small supralinearity starts to appear for doses above 2 Gy (Figure 7.2). For the OSL detected with Hoya U-340 filter we observe a much higher degree of supralinearity (Figure 7.2a) than for OSL detected with combination of Hoya U-340 and Schott WG-360 filters (Figure 7.2c). The data for H 1000 MeV goes only up to
10 Gy due to beam time limitations.

Note that the OSL response to beta rays and H 1000 MeV is similar, regardless of the detection filter (Figure 7.2). The similarity is an indication that the pattern of energy deposition for both types of radiation is similar. Thus, the high energy H 1000 MeV beam deposit most of the energy through high-energy secondary electrons, while the local dose close to the particle tracks is not high enough to reach the saturation level of the detector.

Yukihara and McKeever (2006b) showed that the UV emission band is responsible for the supralinearity in the OSL dose response of Luxel™ detectors. This work extends this observation for the H 1000 MeV beam, and shows that we can avoid the supralinearity of the dose response to H 1000 MeV using a filter combination that blocks the UV emission band of Al₂O₃:C.

For heavier particles, from He to Fe, the OSL response was linear over the investigated dose range. In the case of Fe 200 MeV/u ion, the dose response was linear up to saturation (Figure 7.8). In addition, the dose response is unaffected by the choice of detection filters.

For high-LET radiation the OSL signal can be attributed to individual tracks characterized by similar spatial pattern of energy deposition. Therefore, the ionization density pattern is unchanged by the increase in dose, i.e. particle fluence. Consequently, the OSL signal is linear. As the fluence increases the average distance between adjacent tracks decreases. For larger fluences, interaction between tracks starts to occur. Consequently, the OSL signal saturates. Thus, the luminescence saturation occurs when the particle fluence or dose is high enough for the tracks to start interacting, in the case of the Fe 200 MeV/u beam at around (50-100) Gy (Sawakuchi et al., 2007a). In contrast, ionizing radiation creates luminescence recombination centers in LiF, and HCP track interaction causes supralinearity in the TL response (Horowitz et al., 2001).
Figure 7.2: OSL dose response and luminescence response function of Luxel™ irradiated with H 1000 MeV beam. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) are the beta rays luminescence response functions (see section 3.2).
Figure 7.3: OSL dose response and luminescence response function of Luxel™ irradiated with He 150 MeV/u beam. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) are the beta ray luminescence response functions (see section 3.2).
Figure 7.4: OSL dose response and luminescence response function of Luxel™ detectors irradiated with Ne 400 MeV/u beam. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) are the beta rays luminescence response functions (see section 3.2).
Figure 7.5: OSL dose response and luminescence response function of Luxel\textsuperscript{TM} detectors irradiated with Si 490 MeV/u beam. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) are the beta rays luminescence response functions (see section 3.2).
Figure 7.6: OSL dose response and luminescence response function of Luxel™ detectors irradiated with Fe 1000 MeV/u beam. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) are the beta rays luminescence response functions (see section 3.2).
Figure 7.7: OSL dose response and luminescence response function of Luxel™ detectors irradiated with Fe 500 MeV/u beam. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) are the beta rays luminescence response functions (see section 3.2).
Figure 7.8: OSL dose response and luminescence response function of Luxel™ detectors irradiated with Fe 200 MeV/u beam. a) and b) OSL measured with Hoya U-340 filter (F-center and UV emission bands), and c) and d) OSL measured with combination of Schott WG-360 and Hoya U-340 filters (F-center emission band). The dashed lines in a) and c) represent the linearity, and the full lines in b) and d) are the beta rays luminescence response functions (see section 3.2).
7.2 DEPENDENCE ON IONIZATION DENSITY

The shape of the OSL curve from Al$_2$O$_3$:C depends on ionization density (Yasuda et al., 2002; Yukihara et al., 2004a,b; Gaza et al., 2004, 2006b,a). This section presents a detailed study of the OSL curve shape dependence for nine radiation fields (gamma ray from a $^{60}$Co source, beta ray from a $^{90}$Sr/$^{90}$Y source, H 1000 MeV, He 150 MeV/u, Ne 400 MeV/u, Si 490 MeV/u, Fe 1000 MeV/u, Fe 500 MeV/u and Fe 200 MeV/u).

To improve the comparison between OSL curve shapes, three OSL curves were averaged, the background signal (averaged OSL curves as the average of the last ten points in the OSL curve) was subtracted, and the OSL intensity was divided by its initial intensity.

7.2.1 OSL CURVES FOR DIFFERENT RADIATION QUALITIES AT LOW DOSES

Figures 7.9a and 7.9b show the shape of the OSL curves of Luxel™ detectors when detecting a combination of F-center and UV emission bands, or only F-center emission band for nine different radiation qualities, but the same dose of 100 mGy. The shape of the OSL curves is identical for gamma, beta and H 1000 MeV low LET radiations. As the LET increases the OSL curve becomes faster. Except for the He 150 MeV/u beam, all the other OSL curves have similar shape.

We considered the HCP absorbed dose delivered to the detectors to be equal to:

$$D_{HCP} = \frac{\Phi L_m^\infty}{\rho_m}$$  \hspace{1cm} (7.1)

Note that when delivering the same absorbed dose with HCPs that have different LETs, the fluences of the HCPs are different. For example, the LET of the H 1000 MeV beam is three orders of magnitude lower than the LET of the Fe 200 MeV/u beam. Thus, to deliver the same absorbed dose of H 1000 MeV and Fe 200 MeV/u, the fluence of the H 1000 MeV beam needs to be three orders of magnitude larger than the fluence of the Fe 200 MeV/u beam. Therefore, it is also relevant to study the effect of the different radiation qualities.
Figure 7.9: OSL curve shape of Luxel™ detectors irradiated with gamma of $^{60}$Co source, beta of $^{90}$Sr/$^{90}$Y, H 1000 MeV, He 150 MeV/u, Ne 400 MeV/u, Si 490 MeV/u, Fe 1000 MeV/u, Fe 500 MeV/u and Fe 200 MeV/u. For all OSL curves the same nominal dose of 100 mGy was delivered to the detector. a) OSL measured with Hoya U-340 filter detecting both F-center and UV emission bands, and b) OSL measured with combination of Schott WG-360 and Hoya U-340 filters detecting F-center emission band.
when the same low fluence of HCP is delivered.

Figure 7.10 shows the normalized OSL curves of Luxel™ detectors irradiated with approximately the same low fluence, but different particles and energies. The fluences and corresponding absorbed doses are given in the caption of Figure 7.10. The shape of the OSL curves is similar to the detectors irradiated with the same dose (Figure 7.9). This result is expected because, for low fluences, the HCP tracks are independent from each other.

### 7.2.2 OSL CURVES FOR DIFFERENT ABSORBED DOSES BUT SAME RADIATION QUALITY

We irradiated the detectors with different absorbed doses from the same radiation quality to determine the role of track overlap in the OSL curves.

Figure 7.11 presents normalized OSL curves of Luxel™ detectors exposed to beta ray radiation. For absorbed doses larger than about 10 Gy, the OSL curves decay faster; the higher the dose, the faster the decay. For absorbed doses above 900 Gy the OSL curves present the same shape.

For the Ne 400 MeV/u and Fe 200 MeV/u beams the OSL curves are constant up to a dose of about 50 Gy, starting to decay faster for higher doses until the maximum dose investigated (Figures 7.12 and 7.13). In addition, for the same dose, the OSL curves after HCP irradiation decay faster than the beta irradiated OSL curve, as indicated by the smaller area under the normalized OSL curves (see insets in Figures 7.11, 7.12 and 7.13).

Further changes in the OSL curve occur for a higher value of HCP absorbed dose (50 Gy) compared to beta radiation (10 Gy, see Figure 7.11). We attribute this effect to the fact that, in this case, changes in the OSL curve start only when track overlap becomes important.

We use analytical models of RDD to show that track overlap plays an important role on the changes of the OSL curve of Luxel™ detectors irradiated with HCP. Considering that
Figure 7.10: OSL curve shape of Luxel™ detectors irradiated with H 1000 MeV, He 150 MeV/u, Ne 400 MeV/u, Fe 1000 MeV/u, Fe 500 MeV/u and Fe 200 MeV/u with approximately the same particle fluences. The particle fluences were: $2.79 \times 10^7$ cm$^{-2}$, $2.79 \times 10^7$ cm$^{-2}$, $1.99 \times 10^7$ cm$^{-2}$, $2.06 \times 10^7$ cm$^{-2}$, $3.13 \times 10^7$ cm$^{-2}$ and $2.90 \times 10^7$ cm$^{-2}$, respectively. The absorbed doses in water were: 10 mGy, 100 mGy, 1 Gy, 5 Gy, 10 Gy and 20 Gy, respectively. A) OSL measured with Hoya U-340 filter detecting both F-center and UV emission bands, and B) OSL measured with combination of Schott WG-360 and Hoya U-340 filters detecting F-center emission band.
Figure 7.11: Normalized OSL curves of Luxel\textsuperscript{TM} detectors irradiated with beta rays. a) OSL measured with Hoya U-340 filter detecting both F-center and UV emission bands, and b) OSL measured with combination of Schott WG-360 and Hoya U-340 filters detecting F-center emission band. The insets represent the total area under the normalized OSL curves as a function of absorbed dose.
Figure 7.12: Normalized OSL curves of Luxel™ detectors irradiated with Ne 400 MeV/u beam. a) OSL measured with Hoya U-340 filter detecting both F-center and UV emission bands, and b) OSL measured with combination of Schott WG-360 and Hoya U-340 filters detecting F-center emission band. The insets represent the total area under the normalized OSL curves as a function of absorbed dose.
Figure 7.13: Normalized OSL curves of Luxel™ detectors irradiated with Fe 200 MeV/u beam. a) OSL measured with Hoya U-340 filter detecting both F-center and UV emission bands, and b) OSL measured with combination of Schott WG-360 and Hoya U-340 filters detecting F-center emission band. The insets represent the total area under the normalized OSL curves as a function of absorbed dose.
the HCP beam is randomly distributed over the surface of the detector, the average distance \( d \) between the center of two adjacent tracks can be estimated as

\[
d = 2\sqrt{\frac{1}{\pi\Phi}} \tag{7.2}
\]

where \( \Phi \) is the particle fluence. If \( D(r) \) is the RDD around the center of the track, and if there is track overlap, the distance \( r = d/2 \) is the point where the radial dose \( D(r) \) has its smallest value \( D_{\text{min}} \) (Figure 7.14).

![Figure 7.14: Illustration of overlap between HCP tracks when considering that the tracks are parallel and randomly distributed. \( D(r) \) is a schematic representation of the RDD, \( d \) is the mean distance between two tracks, and \( r = d/2 \) is the middle point between two tracks where the accumulated radial dose \( D(r) \) has its minimum value \( D_{\text{min}} \).](image)

Figure 7.15 shows Fe 200 MeV/u RDDs for 1 Gy, 10 Gy and 50 Gy in Al\(_2\)O\(_3\):C to illustrate the effect of track overlap in the inter-track regions. At low fluences the tracks are far away from each other and the dose level in the inter-track region is very low. As the fluence increases the average distance between adjacent tracks decreases and the dose level in the inter-track region increases.

Considering 50 Gy the HCP dose in which track overlap starts to affect the shape of the OSL curves, we estimated the mean distances \( d \) between two tracks using eq. 7.2. Using different RDD models (chapter 4) we then, estimated the absorbed dose to water \( D_{\text{min}} \) at \( r = d/2 \), the middle distance between two tracks (Figure 7.14). Table 7.1 summarizes the
obtained values of $D_{\text{min}}$. The doses $D_{\text{min}}$ (Table 7.1) are an underestimation because the model is one-dimensional.

Table 7.1 shows that the doses $D_{\text{min}}$ obtained with various models are comparable to the experimental beta dose of about (1-10) Gy above which the OSL curve starts to decay faster. The dose level in the inter-track region where there is overlap of the delta rays dictates the behavior of the OSL curves: as the HCP dose increases above 50 Gy, the local dose in the region between the tracks rises above the (1-10) Gy level, and the OSL curve shape presents further changes. Therefore, the order of magnitude agreement between the inter-track dose $D_{\text{min}}$ and the beta rays dose in which the OSL curve changes is an indication that the macroscopic effect represented by the onset of further changes in the OSL curves for HCP irradiation is due to track overlap (Sawakuchi et al., 2007b).
Table 7.1: Absorbed dose to water and fluence in which the OSL curves start to change, distance \( r = d/2 \), and accumulated minimum absorbed dose to water \( D_{\text{min}} \) at the distance \( r = d/2 \) from the center of the track for Ne 400 MeV/u and Fe 200 MeV/u beams. We calculated \( D_{\text{min}} \) using Chatterjee and Schaefer, Butts and Katz, Kiefer and Straaten, and Geiß et al. models of RDD (see chapter 4).

<table>
<thead>
<tr>
<th></th>
<th>Ne 400 MeV/u</th>
<th>Fe 200 MeV/u</th>
</tr>
</thead>
<tbody>
<tr>
<td>OSL curve change</td>
<td>( \sim 50 \text{ Gy} )</td>
<td>( \sim 50 \text{ Gy} )</td>
</tr>
<tr>
<td>Fluence (( \phi ))</td>
<td>( 9.90 \times 10^8 \text{ cm}^{-2} )</td>
<td>( 7.23 \times 10^7 \text{ cm}^{-2} )</td>
</tr>
<tr>
<td>( r = d/2 )</td>
<td>179 nm</td>
<td>663 nm</td>
</tr>
<tr>
<td>Chatterjee and Schaefer</td>
<td>( D_{\text{min}} = 2.3 \text{ Gy} )</td>
<td>( D_{\text{min}} = 2.4 \text{ Gy} )</td>
</tr>
<tr>
<td>Butts and Katz</td>
<td>( D_{\text{min}} = 1.6 \text{ Gy} )</td>
<td>( D_{\text{min}} = 1.8 \text{ Gy} )</td>
</tr>
<tr>
<td>Kiefer and Straaten</td>
<td>( D_{\text{min}} = 2.7 \text{ Gy} )</td>
<td>( D_{\text{min}} = 3.0 \text{ Gy} )</td>
</tr>
<tr>
<td>Geiß et al.</td>
<td>( D_{\text{min}} = 2.5 \text{ Gy} )</td>
<td>( D_{\text{min}} = 2.8 \text{ Gy} )</td>
</tr>
</tbody>
</table>

7.3 RELATIVE LUMINESCENCE EFFICIENCY OF LUXEL™ DETECTORS

This section presents the values of \( \eta_{\text{HCP,}\gamma} \) from Luxel™ detectors irradiated with the beams presented in Table 6.2. Appendix A presents a complete table with all \( \eta_{\text{HCP,}\gamma} \) data that includes different types of detectors and readout methods.

The procedure used to calculate the \( \eta_{\text{HCP,}\gamma} \) consisted of: (i) readout of the luminescence signal \( S \) from a detector irradiated with the HCP nominal absorbed dose to water \( D_{\text{HCP}} \), measured at the irradiation facility; (ii) using the calibration method described in section 6.3 we determined the detector response \( D \) correspondent to the signal \( S \). \( D \) is the gamma dose that produces the same signal of a detector irradiated with \( D_{\text{HCP}} \). Thus, eq. 3.4 takes the form

\[
\eta_{\text{HCP,}\gamma} = \frac{(S/S_\gamma)D_\gamma}{D_{\text{HCP}}} = \frac{D}{D_{\text{HCP}}} \quad (7.3)
\]

(iii) we subtracted the absorbed dose \( D_c \) received during transportation and storage of the detectors after the HCP irradiations, which was obtained by control detectors, from the response \( D \) to obtain the response due to the HCP irradiations only

\[
\eta_{\text{HCP,}\gamma} = \frac{D - D_c}{D_{\text{HCP}}} \quad (7.4)
\]
For convenience, the doses are absorbed doses to water.

### 7.3.1 BARE BEAM DATA

We determined the experimental $\eta_{HCP,\gamma}$ values (eq. 7.4) in the linear range of the dose response curve, typically the HCP doses were in the interval from 50 mGy to 300 mGy. The only exception was the $\eta_{HCP,\gamma}$ for the Ti 1000 MeV/u irradiation, determined for a nominal absorbed dose of 5 Gy. Although, we did not have dose response curves for the Ti 1000 MeV/u beam, for the dose of 5 Gy we calculated the accumulated minimum inter-track absorbed dose to water $D_{\text{min}}$, as performed for the Fe 200 MeV/u and Ne 400 MeV/u beams (see Table 7.1), and concluded that it is only $D_{\text{min}} = 0.24$ Gy. Furthermore, we showed that the response of LuxelTM detectors is linear up to 50 Gy for high LET particles (Figure 7.8). Thus, we assumed that the Ti 1000 MeV/u dose response is linear at 5 Gy.

Figure 7.16 shows the $\eta_{HCP,\gamma}$ of LuxelTM detectors for OSL measured with Hoya U-340 filter (Figure 7.16a), and a combination of Schott WG-360 and Hoya U-340 filters (Figure 7.16b). The $\eta_{HCP,\gamma}$ values are constant for particles with low-LET, present a region of decreasing $\eta_{HCP,\gamma}$ values as a function of LET, and stabilize for $L_{H_2O}$ higher than around 200 keV/µm. The decreasing $\eta_{HCP,\gamma}$ values as a function of LET is a common trend also observed in other TLD materials such as Al$_2$O$_3$:C single crystals, TLD-100 (see Table A.1) and CaF$_2$:Tm (TLD-300) (Horowitz, 1981).

Appendix A presents a table with the $\eta_{HCP,\gamma}$ data from LuxelTM detectors. Each datum is the average of three measurements and the error represents one experimental standard deviation. In addition, we also present OSL and TL data from Al$_2$O$_3$:C single crystals and TLD-100.

Previous observations showed that the $\eta_{HCP,\gamma}$ from LuxelTM detectors depends on the readout technique and detection filters (Yukihara et al., 2006). Table A.1 and Figure 7.16 show that the use of different detection windows when measuring the OSL from LuxelTM detectors yields different values of $\eta_{HCP,\gamma}$. Thus, our results support previous observations.
Figure 7.16: $\eta_{HCP,\gamma}$ calculated in water of Luxel™ detectors exposed to 24 different combinations of particles and energies. We considered the OSL signal equal to the total area under the OSL curve. a) OSL measured with Hoya U-340 filter detecting both F-center and UV emission bands, and b) OSL measured with combination of Schott WG-360 and Hoya U-340 filters detecting F-center emission band. Red lines are arbitrary functions that fit the data for better visualization.
that the $\eta_{\text{HCP},\gamma}$ in $\text{Al}_2\text{O}_3:\text{C}$ is ultimately characterized by the behavior of the point defects responsible for the detected luminescence signal (Yukihar a et al., 2004a).

Figure 7.17 shows the luminescence response function $f(D)$ to low LET beta radiation (Figure 7.17a), and $\eta_{\text{HCP},\gamma}$ versus $L_\infty$ in water (Figure 7.17b). We observe larger supralinearity and larger values of $\eta_{\text{HCP},\gamma}$ for OSL measured with Hoya U-340 filter compared to the supralinearity and $\eta_{\text{HCP},\gamma}$ values for OSL measured with combination of Hoya U-340 and Schott WG-360 filters. Thus, for OSL measured with Hoya U-340 filter the larger $\eta_{\text{HCP},\gamma}$ values correlate with the larger supralinearity in the dose response function compared to the OSL measured with combination of Hoya U-340 and Schott WG-360 filters.

### 7.3.2 BINARY FILTER DATA

We placed binary filters of known thicknesses and materials between the primary beam and the detectors to decrease the energy of the following primary beams: H 40 MeV, He 150 MeV/u, Ne 400 MeV/u and Si 490 MeV/u.

Figure 7.18 presents the $\eta_{\text{HCP},\gamma}$ of Luxel™ detectors obtained using this approach. The data in Figure 7.18 shows that the $\eta_{\text{HCP},\gamma}$ decreases much faster as a function of LET when compared to the data for bare beams showed in Figure 7.16. Also, we note that the $\eta_{\text{HCP},\gamma}$ versus LET does not obey a single curve.

The HCP creates a pattern of energy deposition around its track that is characteristic of the HCP charge and energy. Thus, particles with the same LET, but different charges and energies create different patterns of energy deposition. As an example, we performed Monte Carlo simulations with the code GEANT4 in $\text{Al}_2\text{O}_3:\text{C}$, density 3.97 g/cm$^3$, with He 9.810 MeV/u ($L_\infty$ in water of 18.76 keV/µm), and O 385.5 MeV/u ($L_\infty$ in water of 19.84 keV/µm) which present approximately the same LET, but different charges and energies. Although the total energy transferred per path length is approximately the same for both particles (same LET), Figure 7.19 shows that the pattern the energy is distributed around the path of the HCPs is completely different.
Figure 7.17: a) Luminescence response function of Luxel™ detectors irradiated with beta rays. b) $\eta_{HCP,\gamma}$ versus $L_\infty$ in water of Luxel™ detectors exposed to different combinations of particles and energies. a) and b) the full symbols represent the OSL detected with Hoya U-340 filters, open symbols represent the OSL detected with combination of Schott WG-360 and Hoya U-340 filters, and full and dashed lines are arbitrary functions fitted to the data for better visualization.
Figure 7.18: $\eta_{\text{HCP,}\gamma}$ calculated in water of Luxel™ detectors. The full line represents the bare beam experimental data. The full symbols represent the bare beam data of the H 40 MeV, He 150 MeV/u, Ne 400 MeV/u and Si 490 MeV/u beams. The open symbols represent data obtained by placing binary filters in front of the H 40 MeV, He 150 MeV/u, Ne 400 MeV/u and Si 490 MeV/u to stop the primary particles. a) OSL detected with Hoya U-340 filter, and b) OSL detected with combination of Schott WG-360 and Hoya U-340 filters.
Figure 7.19: Monte Carlo simulations with GEANT4 in Al$_2$O$_3$:C, density 3.97 g/cm$^3$, with a) and c) He 9.810 MeV/u ($L_\infty$ in water of 18.76 keV/µm); and b) and d) O 385.5 MeV/u ($L_\infty$ in water of 19.84 keV/µm). The number of particles for both beams were 50.

The luminescence of the detectors is intrinsically related to the events of energy deposition. Therefore, different patterns of energy deposition causes different luminescence yields. Figure 7.18 shows that for particles with similar LETs, the particles with lower charge and energy presents lower $\eta_{HCP,\gamma}$. The lower $\eta_{HCP,\gamma}$ is due to a more concentrated spatial pattern of energy deposition.

In summary, this chapter added a significant amount of information on the OSL response of Al$_2$O$_3$:C detectors exposed to HCP, including: i) $\eta_{HCP,\gamma}$ data for 19 new combi-
nations of particles and energies; ii) $\eta_{HCP,\gamma}$ data for various energies of the same particle (H 40 MeV, He 150 MeV/u, Ne 400 MeV/u and Si 490 MeV/u); iii) $\eta_{HCP,\gamma}$ data for different detection windows to study the role of the UV emission band; and iv) detailed study of the luminescence response to different ionization densities and large range of doses and fluences.
CHAPTER 8

PREDICTIONS OF RELATIVE LUMINESCEENCE EFFICIENCY USING THE TRACK STRUCTURE MODEL

This chapter tests the track structure model (TSM) presented in chapter 3 for different RDD analytical models (chapter 4) and simulation (chapter 5). Additionally, we propose a modified version of Butts and Katz model.

As previously discussed, the $\eta_{HCP,\gamma}$ experimental data is usually calculated using values referenced in absorbed dose to water. On the other hand, the TSM leads to $\eta_{HCP,\gamma}$ values based on the absorbed dose in the material. Thus, appropriate comparison between model and experimental data is only possible if we know the conversion factors that transform the $\eta_{HCP,\gamma}$ calculated in the detector’s material to water. Section 8.1 presents a discussion on the definition of the $\eta_{HCP,\gamma}$ and determines the appropriate conversion factors to transform the $\eta_{HCP,\gamma}$ calculated in the detector’s material to $\eta_{HCP,\gamma}$ calculated in water.

Moreover, evaluation of the $\eta_{HCP,\gamma}$ expression obtained through TSM is only possible if we determine the test radiation that reproduces as close as possible the delta ray energy spectrum created by the incident particle. Section 8.2 presents a discussion on the choice of the test radiation for Luxel\textsuperscript{TM} detectors.

Finally, we calculate the $\eta_{HCP,\gamma}$ through the RDD analytical models presented in chapter 4 and simulations presented in chapter 5. Additionally, we introduce a modification of the Butts and Katz model, which improves the predictions of $\eta_{HCP,\gamma}$. 
8.1 RELATIVE LUMINESCENCE EFFICIENCY CALCULATED IN WATER AND IN THE DETECTOR’S MATERIAL

Defining the $\eta_{HCP,\gamma}$ of HCP relative to gamma radiation in terms of the absorbed dose (chapter 3, eq. 3.3), we have:

$$\eta_{HCP,\gamma} = \frac{S_{HCP}(D_{HCP})}{D_{HCP}} / \frac{S_{\gamma}(D_{\gamma})}{D_{\gamma}}$$

(8.1)

where $D_{HCP}$ and $D_{\gamma}$ are absorbed doses in the region where the luminescence signals $S_{HCP}$ and $S_{\gamma}$ of the detector behave linearly. In principle, if no saturation occurs, if $W_{HCP} = W_{\gamma}$, and $\eta_{HCP,\gamma} = 1$, the $\eta_{HCP,\gamma}$ value is unity. This is strictly true only if the absorbed doses $D_{HCP}$ and $D_{\gamma}$ in eq. 8.1 are defined in the material and the dose response is linear. However, the $\eta_{HCP,\gamma}$ is defined in terms of absorbed dose to water, since this quantity is readily available

$$\eta_{H_{2}O, HCP} = \frac{S_{HCP}/D^{H_{2}O}_{HCP}}{S_{\gamma}/D^{H_{2}O}_{\gamma}}$$

(8.2)

The ratio between the relative luminescence efficiencies defined in water and detector’s material is given by

$$\frac{\eta_{H_{2}O, HCP}}{\eta_{m, HCP}} = \frac{D^{H_{2}O}_{\gamma}}{D^{m}_{\gamma}} \times \frac{1/D^{H_{2}O}_{HCP}}{1/D^{m}_{HCP}}$$

(8.3)

The ratio between gamma absorbed doses in different materials is given by the ratio between the mass-energy absorption coefficients $(\mu_{en}/\rho)_{\gamma}^{m}$ of the materials:

$$\frac{D^{H_{2}O}_{\gamma}}{D^{m}_{\gamma}} = \frac{(\mu_{en}/\rho)^{H_{2}O}_{\gamma}}{(\mu_{en}/\rho)^{m}_{\gamma}}$$

(8.4)

On the other hand, the ratio between HCP absorbed doses in different materials is given by the ratio between the material’s density and LET:

$$\frac{1/D^{H_{2}O}_{HCP}}{1/D^{m}_{HCP}} = \frac{\rho_{H_{2}O}/L^{H_{2}O}_{\infty}}{\rho_{m}/L^{m}_{\infty}}$$

(8.5)
Thus, the relationship between $\eta_{HCP,\gamma}$ for absorbed dose to water and absorbed dose to the detector’s material is given by

$$\frac{\eta_{HCP,\gamma}^{H_2O}}{\eta_{HCP,\gamma}^{m}} = \frac{(\mu_{en}/\rho)^{H_2O}_\gamma}{(\mu_{en}/\rho)^{m}_\gamma} \times \frac{\rho_{H_2O}/L_{H_2O}^\infty}{\rho_m/L_{m}^\infty} = \alpha_{m}^{H_2O}(E, L_{H_2O,m}^{H_2O})$$  

(8.6)

where $(\mu_{en}/\rho)^{H_2O}_\gamma$ and $(\mu_{en}/\rho)^{m}_\gamma$ are the mass-energy absorption coefficients in water and in the material of the detector for gamma rays from a $^{60}$Co source, respectively. The ratio between $\eta_{HCP,\gamma}$ calculated in water and in detector’s material is a constant for a given type of particle and energy, and fixed reference radiation field. We call this constant the conversion factor $\alpha_{m}^{H_2O}(E, L_{H_2O,m}^{H_2O})$, where $E$ is the energy of the photon from the reference radiation field. This relationship shows that the $\eta_{HCP,\gamma}$ defined in eq. 8.2 for a “perfect” detector is different from unity (for low-LET radiation in which the luminescence does not saturate in regions close to the path of the incident particle), but depends on the detector’s material. Assuming a $^{60}$Co reference source (mean photon energy of 1.25 MeV) and Al$_2$O$_3$:C as the detector’s material, the ratio between the mass-energy absorption coefficients can be evaluated and the conversion factor $\alpha_{m}^{H_2O}(1.25 \text{ MeV}, L_{H_2O,Al_2O_3:C}^{H_2O})$ become

$$\alpha_{Al_2O_3:C}^{H_2O}(1.25 \text{ MeV}, L_{H_2O,Al_2O_3:C}^{H_2O}) = 1.134 \times \frac{\rho_{H_2O}/L_{H_2O}^\infty}{\rho_{Al_2O_3:C}/L_{Al_2O_3:C}^\infty}$$  

(8.7)

The mass-energy absorption coefficient data were taken from the NIST database (Hubbell and Seltzer, 2004). There are no available mass-energy absorption coefficient data of Al$_2$O$_3$. Thus, we used the data from aluminum and oxygen weighted by the mass fraction of this elements in Al$_2$O$_3$ (Johns and Cunningham, 1983). Table 8.1 shows the conversion factor $\alpha_{Al_2O_3:C}^{H_2O}(1.25 \text{ MeV}, L_{H_2O,Al_2O_3:C}^{H_2O})$ for Al$_2$O$_3$:C detectors and for the particles and energies used in this work, and Figure 8.1 shows the comparison between the $\eta_{HCP,\gamma}$ values calculated in water and Al$_2$O$_3$:C. As an example we consider the H 230 MeV beam in
which

\[ \eta_{HCP,\gamma}^{H_2O} = 0.934 \times \eta_{HCP,\gamma}^{Al_2O_3:C} \]  \hspace{1cm} (8.8)

The dose response function to beta radiation of the F-center emission band in Al₂O₃:C presents only a small supralinearity (Figure 7.1). Thus, we expect \( \eta_{HCP,\gamma}^{Al_2O_3:C} \) values close to unity for low-LET HCP beams, i.e. beams that do not saturate the luminescence of the detector in regions close to the HCP path, such as H 230 MeV. Assuming the OSL \( \eta_{HCP,\gamma}^{Al_2O_3:C} \) equals to unity for low-LET HCP particles, the result of eq. 8.8 for the H 230 MeV beam shows good agreement with the experimental OSL \( \eta_{HCP,\gamma} \) calculated in water of 0.951 ± 0.006 (Table A.1).

The values of OSL \( \eta_{HCP,\gamma} \) larger than unity for Luxel™ detectors calculated in water when detecting both F-center and UV emission bands (Table A.1) are due to the large supralinearity observed in the response function of the detector irradiated with beta radiation (Figure 7.1).

### 8.2 TEST RADIATION TO SIMULATE THE DELTA RAY SPECTRUM

Under conditions of electronic equilibrium, the absorbed dose \( D_m \) in the material \( m \) is (Johns and Cunningham, 1983):

\[ D_m = \Phi \bar{E}_{ab} \left( \frac{\mu_{en}}{\rho} \right)_m \]  \hspace{1cm} (8.9)

where \( \Phi \) is the fluence of photons, \( \bar{E}_{ab} \) is the part of the average kinetic energy transferred to electrons that contribute to ionizations, and \( \left( \frac{\mu_{en}}{\rho} \right)_m \) is the mass-energy absorption coefficient of the material.

For the same type of radiation \( k \) and same photon fluence \( \Phi \), the ratio between the absorbed dose in two different materials is:

\[ \frac{D_{m1}^k}{D_{m2}^k} = \frac{\left( \frac{\mu_{en}}{\rho} \right)_{m1}^k}{\left( \frac{\mu_{en}}{\rho} \right)_{m2}^k} \]  \hspace{1cm} (8.10)
Table 8.1: Conversion factor $\alpha_{H_2O:Al_2O_3:C}^{H_2O} (1.25 \text{ MeV}, L_{\infty}^{H_2O, Al_2O_3:C})$ to transform the $\eta_{HCP,\gamma}$ calculated to Al$_2$O$_3$:C to the one calculated to water or vice-versa.

<table>
<thead>
<tr>
<th>Beam</th>
<th>Energy (MeV/u)</th>
<th>$L_{\infty}$ in H$_2$O (keV/µm)</th>
<th>$L_{\infty}$ in Al$_2$O$_3$:C (keV/µm)</th>
<th>$\alpha_{Al_2O_3:C}^{H_2O}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H 1000 MeV</td>
<td>1000</td>
<td>0.223</td>
<td>0.734</td>
<td>0.943</td>
</tr>
<tr>
<td>H 230 MeV</td>
<td>230</td>
<td>0.413</td>
<td>1.35</td>
<td>0.934</td>
</tr>
<tr>
<td>H 70 MeV</td>
<td>70</td>
<td>0.960</td>
<td>3.10</td>
<td>0.923</td>
</tr>
<tr>
<td>H 40 MeV</td>
<td>40</td>
<td>1.50</td>
<td>4.79</td>
<td>0.910</td>
</tr>
<tr>
<td>H 30 MeV</td>
<td>30</td>
<td>1.90</td>
<td>6.02</td>
<td>0.906</td>
</tr>
<tr>
<td>He 150 MeV/u</td>
<td>144.2</td>
<td>2.24</td>
<td>7.31</td>
<td>0.930</td>
</tr>
<tr>
<td>H 24 MeV</td>
<td>24</td>
<td>2.27</td>
<td>7.19</td>
<td>0.903</td>
</tr>
<tr>
<td>H 20 MeV</td>
<td>20</td>
<td>2.64</td>
<td>8.31</td>
<td>0.900</td>
</tr>
<tr>
<td>H 17 MeV</td>
<td>17</td>
<td>3.01</td>
<td>9.45</td>
<td>0.897</td>
</tr>
<tr>
<td>H 14 MeV</td>
<td>14</td>
<td>3.52</td>
<td>11.02</td>
<td>0.894</td>
</tr>
<tr>
<td>C 400 MeV/u</td>
<td>386.9</td>
<td>11.14</td>
<td>36.52</td>
<td>0.936</td>
</tr>
<tr>
<td>C 290 MeV/u</td>
<td>277.2</td>
<td>13.30</td>
<td>43.51</td>
<td>0.935</td>
</tr>
<tr>
<td>O 1000 MeV/u</td>
<td>1000</td>
<td>14.24</td>
<td>46.97</td>
<td>0.942</td>
</tr>
<tr>
<td>O 400 MeV/u</td>
<td>385.5</td>
<td>19.84</td>
<td>65.03</td>
<td>0.936</td>
</tr>
<tr>
<td>C 135 MeV/u</td>
<td>111.2</td>
<td>24.41</td>
<td>79.28</td>
<td>0.928</td>
</tr>
<tr>
<td>Ne 400 MeV/u</td>
<td>371.9</td>
<td>31.55</td>
<td>103.4</td>
<td>0.937</td>
</tr>
<tr>
<td>Si 490 MeV/u</td>
<td>444.8</td>
<td>56.80</td>
<td>186.4</td>
<td>0.938</td>
</tr>
<tr>
<td>Ar 500 MeV/u</td>
<td>450.7</td>
<td>93.34</td>
<td>306.4</td>
<td>0.938</td>
</tr>
<tr>
<td>Ti 1000 MeV/u</td>
<td>977.6</td>
<td>108.2</td>
<td>356.9</td>
<td>0.942</td>
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<tr>
<td>Fe 1000 MeV/u</td>
<td>967.0</td>
<td>151.4</td>
<td>499.4</td>
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</tr>
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<td>200.3</td>
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<td>0.938</td>
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<td>Fe 200 MeV/u</td>
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<td>431.8</td>
<td>1403</td>
<td>0.928</td>
</tr>
<tr>
<td>Kr 400 MeV/u</td>
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<td>447.2</td>
<td>1464</td>
<td>0.935</td>
</tr>
<tr>
<td>Xe 290 MeV/u</td>
<td>185.5</td>
<td>1368</td>
<td>4462</td>
<td>0.932</td>
</tr>
</tbody>
</table>
Figure 8.1: $\eta_{HCP,\gamma}$ calculated in water and $\text{Al}_2\text{O}_3$ of Luxel$^\text{TM}$ detectors. a) OSL measured with Hoya U-340 filter detecting both F-center and UV emission bands, and b) OSL measured with combination of Schott WG-360 and Hoya U-340 filters detecting F-center emission band. Red lines are arbitrary functions that fit the $\eta_{HCP,\gamma}$ data calculated in water for better visualization.
In medical dosimetry it is common to calibrate the detector against a $^{60}$Co source in absorbed dose to water. Thus,

$$\frac{(D_{m1}/D_{H2O})_k}{(D_{m1}/D_{H2O})_\gamma} = \left[\frac{([\mu_{en}/\rho]_{m1}/([\mu_{en}/\rho]_{H2O})_k}{([\mu_{en}/\rho]_{m1}/([\mu_{en}/\rho]_{H2O})_\gamma}\right]$$  \hspace{1cm} (8.11)

For the same type of radiation and material, the luminescence signal is proportional to the absorbed dose. However, for different radiation types and materials, the partition of absorbed energy through excitations and ionizations varies. Ionizations create free electrons which are trapped in the main dosimetric trap and are responsible for the luminescence. Thus, in luminescence dosimetry the luminescence signal is ultimately proportional to the trapped number of secondary electrons produced by the primary radiation. The luminescence signal $S$ from a detector made of material $m$ exposed to the radiation field $k$ is given by (see eq. 3.11):

$$S^m_k = \alpha \eta_k(D_0) f^m_k(D) D^m_k \rho_m V$$  \hspace{1cm} (8.12)

where $\alpha$ is the efficiency of the experimental apparatus, $\eta_k$ is the luminescence efficiency to the radiation field $k$ for low doses $D_0$, $f^m_k(D)$ is the luminescence response function, $D^m_k$ is the absorbed dose to the material $m$, $\rho_m$ is the density of the material, and $V$ is the irradiated volume.

Usually, the literature compares the luminescence response for different types of radiation relative to the response of a $^{60}$Co source calibrated in absorbed dose to water:

$$\frac{(S/D_{H2O})_k}{(S/D_{H2O})_\gamma} = \eta_{k,\gamma} \left(\frac{D^m_k/D_{H2O}}{D^m_k/D_{H2O}}_\gamma\right)$$  \hspace{1cm} (8.13)

where $\eta_{k,\gamma}$ is the relative luminescence efficiency between the radiation $k$ and gamma. We assume that the dose is in the linear range of the detector’s response, thus, $f(D) = 1$. 

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Substituting eq. 8.11 in eq. 8.13 we have:

\[
\frac{(S/D)_{\text{H}_2\text{O}}}{(S/D)_{\text{H}_2\text{O}}} = \frac{\eta_{k,\gamma}}{\gamma} \left[ \frac{[\mu_{\text{en}}/\rho]^m}{[\mu_{\text{en}}/\rho]^H_{\text{H}_2\text{O}}} \right] k
\]

(8.14)

The detector presents an “anomalous” energy response if the relative response of the detector deviates from the ratio between the mass energy absorption coefficients (eq. 8.14), indicating that the factor \(\eta_{k,\gamma}\) changes with energy and differs from unity. This anomaly was partially explained using the microdosimetric approach (Olko, 2002) as being caused by the ionization density created by different photon energies.

For gases, the average energy required to create an electron pair \(W_k\) strongly increases for electron energies lower than around 1 keV (ICRU, 1979; IAEA, 1995). This increase in \(W_k\) is related to the increase in the energy absorbed through excitations in the partition of absorbed energy through excitations and ionizations (ICRU, 1979; IAEA, 1995). Thus, for low electron energies, the number of secondary electrons created by ionization events is smaller when compared to the high energy case. Indeed, the response of detectors is anomalous only for low energy photons where the contribution of low energy electrons is important to the events of absorption of energy. The luminescence signal is ultimately proportional to the trapped number of secondary electrons produced by the primary radiation. Thus, we suggest that the so-called anomalous response of luminescence detectors is also related to the increasing in the average energy required to create an electron-hole pair, which is implicitly incorporated into \(\eta_{k,\gamma}\) (see eq. 3.21), for low electron energies and consequently decrease in the efficiency in which the primary radiation creates secondary electrons. Unfortunately, the lack of \(W_k\) data for TLD and OSLD materials makes impossible testing our suggestion.

Figure 8.2 presents the ratio of mass-energy absorption coefficients between \(\text{Al}_2\text{O}_3\) and water, normalized to the mean energy of \(^{60}\text{Co}\) gamma rays (1.25 MeV). The data are from the NIST database (Hubbell and Seltzer, 2004). We also plot in Figure 8.2 TL
data for different photon energies from Al\(_2\)O\(_3\):C (Akselrod et al., 1990). The TL data was normalized to the mean energy of \(^{60}\)Co gamma rays.

Figure 8.2: The solid line represents the ratio between the mass-energy absorption coefficients of Al\(_2\)O\(_3\) and water, normalized to the mean energy of \(^{60}\)Co gamma rays. Solid circles represent the relative TL of Al\(_2\)O\(_3\):C normalized to the mean energy of \(^{60}\)Co gamma rays. The TL data are from the literature (Akselrod et al., 1990) and mass-energy absorption coefficient data are from the NIST database (Hubbell and Seltzer, 2004).

Figure 8.2 shows that the TL yield of Al\(_2\)O\(_3\):C follows its mass-energy absorption coefficient for photons with energy larger than 80 keV. Thus, down to 80 keV photons \(\eta_{k,\gamma}\) is approximately equal to unity. For energies lower than 80 keV the TL data is lower than the mass-energy absorption coefficient, indicating that \(\eta_{k,\gamma} < 1\). Data from Olko et al. (2006) and unpublished OSL\(^1\) results show the same behavior.

We now discuss the influences of the TL and OSL anomalous energy dependence on the relative luminescence efficiency formula derived using TSM.

For completeness we rewrite the equation derived in chapter 3 that calculates the \(\eta_{HCP,\gamma}\) using TSM.

\[
\eta_{HCP,\gamma} = \frac{\int_{0}^{R_{\text{Max}}} \eta_{k,\gamma}f_X[D(r)]\rho_mD(r)2\pi r dr}{\int_{0}^{R_{\text{Max}}} \rho_mD(r)2\pi r dr}
\]  

\(\text{8.15}\)

\(^1\)Dr. M. Akselrod personal communication, Landauer, Inc.
where

$$\eta_{\delta,\gamma} = \epsilon'_{\delta,\gamma} \frac{1}{W_{HCP}} \frac{1}{W_{\gamma}}$$  \hspace{1cm} (8.16)$$

$\eta_{HCP,\gamma}$ is the relative luminescence efficiency from the HCP field in respect to gamma radiation from a $^{60}$Co source calculated in the linear range of the dose response curve; $\eta_{\delta,\gamma}$ is the relative luminescence efficiency between secondary electrons and gamma radiation; $\epsilon'_{\delta,\gamma}$ is the ratio between the efficiency to convert the low energy charges created by the HCP and gamma rays into luminescence; $R_{\text{Max}}$ is the maximum radial distance a delta ray can travel; $f_X$ is the response function of the detector to the test radiation field $X$ obtained for doses in the detector’s material; $D(r)$ is the RDD function calculated in the detector’s material; $\rho_m$ is the density of the detector; and $r$ is the radial distance.

The factor $\eta_{\delta,\gamma}$ in eq. 8.15 can be determined from the luminescence response to different photon energies (see eq. 8.14). HCP produces secondary electrons with energies ranging from 0 eV to up to a few MeV, depending on the energy of the HCP. Thus, for accurate determination of $\eta_{HCP,\gamma}$, we must provide $\eta_{\delta,\gamma}$ data for the entire energy spectrum. Indeed, the RDD models show that low energy secondary electrons are responsible for a large part of the dose. Using Butts and Katz model we determined that for a 1000 MeV/u particle about 90% of the secondary electrons have energies lower than 80 keV. Thus, for HCP energies lower than 1000 MeV/u most of the secondary electrons have energies lower than 80 keV, indicating that the Luxel™ detectors are in the anomalous energy response region for all the particles used in this study.

We have only accurate dose response data for beta rays from a $^{90}\text{Sr}^{90}\text{Y}$ source. Thus, we used beta rays as the test radiation. Moreover, to simplify the $\eta_{HCP,\gamma}$ calculations we approximate $\eta_{\delta,\gamma} = 1$ for the entire energy spectrum of the secondary electrons produced by the HCP. We encourage further investigations to determine the best compromise test radiation and the factor $\eta_{\delta,\gamma}$. We consider the use of beta rays as the test and the approximation $\eta_{\delta,\gamma} = 1$ limitations in our approach.

Thus, considering $^{90}\text{Sr}^{90}\text{Y}$ source (calibrated against a $^{60}$Co source) as the test radiation
We explicitly wrote the index Al$_2$O$_3$:C to emphasize that the $\eta_{HCP,\gamma}$ is calculated in the detector’s material. Eq. 8.6 and Table 8.1 provide the ingredients to transform $\eta_{HCP,\gamma}$ calculated in the detector’s material to $\eta_{HCP,\gamma}$ calculated in water. Throughout this chapter all $\eta_{HCP,\gamma}$ values are properly converted into $\eta_{HCP,\gamma}$ values calculated in water.

8.3 RELATIVE LUMINESCENCE EFFICIENCY OBTAINED USING ANALYTICAL MODELS OF RADIAL DOSE DISTRIBUTION

We used the RDD analytical models presented in chapter 4 together with eq. 8.17 to calculate $\eta_{HCP,\gamma}$. To evaluate eq. 8.17 we first converted the OSL dose response versus absorbed dose to water (Figure 7.1) to the OSL dose response versus absorbed dose to Al$_2$O$_3$:C using the ratio between the mass-energy absorption coefficients in water and Al$_2$O$_3$ for the mean photon energy of 1.25 MeV for a $^{60}$Co source:

$$\frac{D_{Al_2O_3}}{D_{H_2O}} = \frac{(\mu/\rho)_{Al_2O_3}}{(\mu/\rho)_{H_2O}} = 0.882$$ (8.18)

The response functions from Luxel™ detectors for absorbed dose to Al$_2$O$_3$:C when detecting F-center and UV emission bands (Hoya U-340 filter), and when detecting F-center emission band only (Hoya U-340 and Schott WG-360 filters) were parameterized with the following expression:

$$f^A_{\beta Al_2O_3:C}(D) = \frac{(1 - e^{-A_0D})}{(A_0D)} + \frac{A_1(1 - e^{-A_2D^{A_3}})}{(A_0D)}$$ (8.19)

Table 8.2 gives the parameters $A_0$, $A_1$, $A_2$ and $A_3$ for each detection window and Figure 8.3 shows the experimental data and the fitted functions.
Table 8.2: Values of the parameters $A_0$, $A_1$, $A_2$ and $A_3$ from the fitting of the response function versus absorbed dose to $\text{Al}_2\text{O}_3$:C (eq. 8.19).

<table>
<thead>
<tr>
<th>parameter</th>
<th>Luxel\textsuperscript{TM} detector</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>U-340 (F-center and UV emission)</td>
</tr>
<tr>
<td>$A_0$ ($\text{Gy}^{-1}$)</td>
<td>$4.52 \times 10^{-3} \pm 0.39 \times 10^{-3}$</td>
</tr>
<tr>
<td>$A_1$</td>
<td>$5.35 \times 10^{-1} \pm 0.75 \times 10^{-1}$</td>
</tr>
<tr>
<td>$A_2$ ($\text{Gy}^{-A_3}$)</td>
<td>$1.04 \times 10^{-3} \pm 0.08 \times 10^{-3}$</td>
</tr>
<tr>
<td>$A_3$</td>
<td>$1.57 \pm 0.02$</td>
</tr>
</tbody>
</table>

Figure 8.3: Luminescence response function of Luxel\textsuperscript{TM} detectors for absorbed dose to $\text{Al}_2\text{O}_3$:C. Full circles represent the data when detecting both F-center and UV emission bands. Empty squares represent the data when detecting only F-center emission band. Full and dashed lines represent the fitting to the data when detecting both F-center and UV emission bands, and only F-center emission band, respectively.
Substituting eq. 8.19 in eq. 8.17 we obtain the final expression used to calculate the \( \eta_{HCP,\gamma} \):

\[
\eta^{Al_2O_3:C}_{HCP,\gamma} = \frac{2\pi \rho_{Al_2O_3:C}}{A_0 L_\infty^{Al_2O_3:C}} \int_0^{R_{max}} \left[ (1 - e^{-A_0 D(r)}) + A_1 (1 - e^{-A_2 D(r)^3}) \right] r dr
\]  

(8.20)

where \( D(r) \) is the RDD model, and the integral was numerically evaluated using Maple 10 (Maplesoft\textsuperscript{TM}, 2005). Finally, we converted \( \eta^{Al_2O_3:C}_{HCP,\gamma} \) calculated in \( Al_2O_3:C \) by eq. 8.20 to \( \eta_{HCP,\gamma} \) calculated in water.

We represented the comparison between the \( \eta_{HCP,\gamma} \) data and the modeling in terms of the percentage deviation:

\[
\% = \left[ 1 - \frac{\eta_{HCP,\gamma}(Exp.)}{\eta_{HCP,\gamma}(Model)} \right] \times 100
\]  

(8.21)

Figures 8.4 and 8.5 present the comparison between \( \eta_{HCP,\gamma} \) experimental data and modeling according to eq. 8.21. We included in Figures 8.4 and 8.5 only particles with range in \( Al_2O_3:C \) about three times larger than the thickness of the detector so that the approximation of constant LET is valid. Note that none of the models agree with experimental data in the whole range of LET. Different RDD analytical models lead to different predictions of \( \eta_{HCP,\gamma} \). For \( L_{H_2O}^{H_2O} \) lower than around 100 keV/\( \mu \)m, the Chatterjee and Schaefer, Waligórski \textit{et al.} and Fageeha \textit{et al.} models overestimate the experimental data to about 50 \%. For \( L_{H_2O}^{H_2O} \) larger than around 10 keV/\( \mu \)m, Butts and Katz, Kiefer and Straaten, and Geiß \textit{et al.} models underestimate the experimental data to about 80 \%.

From the calculations of OSL \( \eta_{HCP,\gamma} \) using the RDDs of Chatterjee and Schaefer, Butts and Katz, Waligórski \textit{et al.}, Fageeha \textit{et al.}, Kiefer and Straaten, and Geiß \textit{et al.} models we conclude that improvements needed to be done since the predictions present up to 80 \% disagreement from data for the particles and energies of interest.
Figure 8.4: Comparison between OSL $\eta_{\text{HCP,} \gamma}$ experimental data and modeling using the RDD functions from Chatterjee and Schaefer, Butts and Katz, Waligórski et al. and Fageeha et al. models. The figures in the left side present the comparison for OSL detected with Hoya U-340 filters (F-center and UV emission bands), and the figures in the right side for OSL detected with Hoya U-340 and Schott WG-360 (F-center emission band).
Figure 8.5: Comparison between OSL $\eta_{HCP,\gamma}$ experimental data and modeling using the RDD functions from Kiefer and Straaten, and Geiß et al. models. The figures in the left side present the comparison for OSL detected with Hoya U-340 filters (F-center and UV emission bands), and the figures in the right side for OSL detected with Hoya U-340 and Schott WG-360 (F-center emission band).
8.4 IMPROVEMENT OF BUTTS AND KATZ MODEL OF RADIAL DOSE DISTRIBUTION AND DETERMINATION OF RELATIVE LUMINESCENCE EFFICIENCY

Butts and Katz model of RDD uses the Rutherford’s SDCS for production of secondary electrons. As discussed in section 4.2, Rutherford’s formula considers only the ionization energy, excluding excitation energy. Therefore, estimation of the total energy transferred per path length (LET) leads to incorrect values.

Waligórski et al. (1986) and Fageeha et al. (1993) improved the estimation of LET by multiplying the RDD function derived in the Butts and Katz model by an arbitrary function, as discussed in section 4.2.

This section presents a modified version of the Butts and Katz model. We introduce a constant region of energy deposition for small radial distances. This constant region is similar to the definition of core in the Chatterjee and Schaefer, and Geiß et al. models. We determine the core region normalizing the total energy loss per path length to the LET of the particle. Hansen and Olsen (1984) used similar approach.

We modify Butts and Katz model adding a constant term representing the energy transferred by excitation and ionization. The final equation then becomes:

\[
D(r) = \begin{cases} 
  k, & 0 < r < r_c \\
  \frac{N_c e^4 Z^2}{m_e c^2 \alpha \beta^2} \frac{1}{r} \left[ \frac{1 - \frac{r + r_0}{R_{Max} + r_0}}{r + r_0} \right]^{1/\alpha}, & r_c < r < R_{Max} 
\end{cases}
\]  

(8.22)

where \( r_0 \) is given by eq. 4.27, \( R_{Max} \) is parameterized as

\[
R_{Max} = \frac{6.24 \times 10^6}{\rho_m} \left( \frac{\beta^2}{\kappa - \beta^2} \right)^{1.667}
\]  

(8.23)

where \( \kappa = 1.5 \) was determined by adjusting the relative luminescence efficiency values to
the experimental data.

The constant $k$ is determined by normalizing the total energy loss per path length to the LET of the particle:

$$2\pi \int_0^{R_{\text{Max}}} r D(r) \, dr = \frac{L_m^m}{\rho_m}$$

(8.24)

We parameterize the radius of the core $r_c$ using a function of the form:

$$r_c = A(1 - e^{-B \frac{Z^*}{\sigma^*}})$$

(8.25)

where we determine the constants $A$ and $B$ adjusting their values to fit three values of $\eta_{\text{HCP,}\gamma}$ data from Luxel™ detectors when F-center emission band is detected (Table A.1) – one value for low LET particle, one value in the intermediate range of LET and one value for high LET particle. Thus, we determine $A = 47.3$ nm, and $B = 0.145$.

To choose the form of the function 8.25, we consider that the core can be approximated by a region that depends not only on the properties of the detector, but also on the strength with which an incident particle can interact with the detector, represented by the saturated exponential term. Thus, the term between parentheses is an intrinsic property of the incident particle, such as charge and speed. The constant $B$ has the same numerical value for all types of detectors. On the other hand, the constant $A$ has dimension of length, relating to physical distances inside of the detector.

We also determined the constant $A$ for the OSL from F-center and UV emission bands. $A$ was determined fixing the value of $B = 0.145$ and adjusting the constant $A$ such that the $\eta_{\text{HCP,}\gamma}$ fits three data points located: one in the low-LET region, one in the intermediate-LET region, and one in the high-LET region. A value of $A = 38.0$ nm was determined. Table 8.3 summarizes the values of the constant $A$ and $B$ for both detection windows.

Figure 8.6 shows RDD in Al$_2$O$_3$:C according to the modified version of Butts and Katz model. Note that the core radius depends on the properties of the defects related to the luminescence process. For comparison we also include in Figure 8.6 the Butts and Katz
Table 8.3: Values of the parameters $A$ and $B$ from eq. 8.25 to make RDD from the modified Butts and Katz model fit data for the two different filter sets.

<table>
<thead>
<tr>
<th>Luxel$^{TM}$ detector</th>
<th>F-center and UV emissions</th>
<th>F-center emission</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>38.0 nm</td>
<td>47.3 nm</td>
</tr>
<tr>
<td>$B$</td>
<td>0.145</td>
<td>0.145</td>
</tr>
</tbody>
</table>

A physical interpretation of the constant $A$ leads to a physical interpretation of the core region. Matter in such small regions can not be consider “continuous” and the definition of dose breaks down. Thus, the RDD core region as defined in our model is not the physical absorbed dose, but is related to the luminescence properties of the detector. It is not the
scope of this work to give a definitive interpretation of such region, but we would like to make comparisons between the determined $A$ values in Luxel\textsuperscript{TM} detectors and distances between the luminescence centers that take place in the OSL process in Al\textsubscript{2}O\textsubscript{3}:C.

Luxel\textsuperscript{TM} detectors are made of Al\textsubscript{2}O\textsubscript{3}:C crystals in powder form. The luminescence centers responsible for the OSL process in Al\textsubscript{2}O\textsubscript{3}:C are the F-center and F\textsuperscript{+}-center, plus an unknown center with emission centered at 334 nm (see chapter 2). The concentration of F\textsuperscript{+}-centers in non-irradiated Al\textsubscript{2}O\textsubscript{3}:C crystals used to make the Luxel\textsuperscript{TM} detectors is in the interval between $0.5 \times 10^{15}$ cm\textsuperscript{-3} and $2.0 \times 10^{15}$ cm\textsuperscript{-3}. The concentration of F-centers is about one order of magnitude higher than the concentration of F\textsuperscript{+}-centers (Akselrod et al., 1993). By the concentration of centers, we estimate the average distance between defects to be in the range between 79 nm and 126 nm for F\textsuperscript{+}-centers, and in the range between 37 nm and 58 nm for F-centers.

The value of $A = 47.3$ nm obtained when detecting only F-center emission band is within the calculated (37-58) nm interval of the average distance between F-centers in Luxel\textsuperscript{TM} detectors. Furthermore, for the OSL when detecting F-center and UV emission bands, in addition to the F-center, another unknown defect participates in the OSL process. In this case, the total concentration of defects participating in the OSL process is higher and the average distance between defects that participate in the OSL process is smaller than the case when detecting only the F-center emission band. Indeed, a lower value of $A = 38.0$ nm is obtained when detecting F-center and UV emission bands, correlating to the larger concentration of defects participating in the OSL process.

Although we observe a correlation between the maximum size of the core radius and the average distance between F-centers in Al\textsubscript{2}O\textsubscript{3}:C, we do not claim that this is a definitive physical interpretation. The definition of the core region presented in this subsection was with the purpose of finding a parameter that can be adjusted to improve the prediction of $\eta_{\text{HCP,}\gamma}$ in Luxel\textsuperscript{TM} detectors.

\textsuperscript{2}M. Akselrod, personal communication, Landauer Inc.
Figure 8.7 shows the comparison between the $\eta_{HCP,\gamma}$ calculated using the RDD from the modified version of the Butts and Katz model and experimental data for the bare beam irradiations. In Figure 8.7 the arrows indicate the data points used to find the parameters $A$ and $B$ for the core radius, and the insets represent the difference between experimental data and modeling according to eq. 8.21. Agreement within 15 % is observed when F-center and UV emission bands are detected and within 20 % when F-center emission band is detected.

For the irradiations placing binary filters in front of the bare beam, the agreement between the experimental data and modeling is within 35 % when F-center and UV emission bands are detected and within 35 % when F-center emission band is detected (Figure 8.8). Note that the predictions are inaccurate for the proton beam and also for the last points of each beam. This deviation is because these particles have low energies and they can not be considered to have a constant LET inside of the detector. To accurately apply the calculations of $\eta_{HCP,\gamma}$ using the model presented in this work the $\eta_{HCP,\gamma}$ expression needs to be modified to include the LET variation for particles that stop inside of the detector.

Table 8.4 and Table 8.5 show the experimental data and the calculated $\eta_{HCP,\gamma}$ determined in water for all the RDD models. Table 8.4 presents the $\eta_{HCP,\gamma}$ values of Luxel™ detectors measuring both F-center and UV emission bands (Hoya U-340 filter), and Table 8.5 presents the $\eta_{HCP,\gamma}$ values measuring only F-center emission band (Hoya U-340 and Schott WG-360 filters). In Table 8.4 and Table 8.5 we also included the calculated values of $\eta_{HCP,\gamma}$ for particles and energies in which the approximation of constant LET of the particle is invalid.

In summary, the modeling shows results in agreement within 20 % of experimental data for particles that have constant LET when passing through the detector, and with charges up to 54 and $L_\infty$ in water up to 1368 keV/µm.

The model presented in this section has the radius of the core as a free parameter, which is determined by fitting the constant $A$ in eq. 8.25 to the $\eta_{HCP,\gamma}$ data – at least three points
Figure 8.7: Comparison between $\eta_{HCP,\gamma}$ experimental data and modeling using the RDD functions from a modified version of Butts and Katz model. The arrows indicate the data points used to find the parameters $A$ and $B$ for the core radius. The insets represent the percentage deviation between data and model. a) OSL from Luxel™ detected with Hoya U-340 filters (F-center and UV emission bands); b) OSL from Luxel™ detected with Hoya U-340 and Schott WG-360 (F-center emission band).
Figure 8.8: Comparison between $\eta_{HCP,\gamma}$ experimental data and modeling using the RDD functions from a modified version of Butts and Katz model. The experimental data was obtained by placing binary filters in front of the H 40 MeV, He 150 MeV/u, Ne 400 MeV/u, and Si 490 MeV/u to stop the primary particles. The full lines represent the results from the modeling, and symbols the experimental data. The insets represent the percentage deviation between data and model. a) OSL from Luxel$^{\text{TM}}$ detected with Hoya U-340 filter (F-center and UV emission bands); b) OSL from Luxel$^{\text{TM}}$ detected with Hoya U-340 and Schott WG-360 filters (F-center emission band).
Table 8.4: Modeling of OSL $\eta_{HCP,\gamma}$ of Luxel$^{TM}$ detectors detecting both F-center and UV emission bands (Hoya U-340 filter). We obtained the $\eta_{HCP,\gamma}$ values through TSM using different RDD analytical models and MC simulations with GEANT4. The $\eta_{HCP,\gamma}$ values are calculated in water.

<table>
<thead>
<tr>
<th>Beam</th>
<th>Energy (MeV/u)</th>
<th>$L_{H2O}^{\infty}$ (keV/µm)</th>
<th>Experimental data</th>
<th>Chatterjee</th>
<th>Katz</th>
<th>Waligórska</th>
<th>Fageeha</th>
<th>Geiß</th>
<th>Kiefer</th>
<th>Katz-Core (This work)</th>
<th>GEANT4 (This work)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H 1000 MeV</td>
<td>1000</td>
<td>0.223</td>
<td>1.022 ± 0.174</td>
<td>0.973</td>
<td>0.968</td>
<td>0.1.111</td>
<td>0.928</td>
<td>0.904</td>
<td>0.859</td>
<td>1.155</td>
<td>1.119</td>
</tr>
<tr>
<td>H 230 MeV</td>
<td>230</td>
<td>0.413</td>
<td>1.021 ± 0.003</td>
<td>0.643</td>
<td>0.943</td>
<td>0.971</td>
<td>0.791</td>
<td>0.868</td>
<td>0.799</td>
<td>1.175</td>
<td>1.097</td>
</tr>
<tr>
<td>H 70 MeV</td>
<td>70</td>
<td>0.960</td>
<td>1.016 ± 0.117</td>
<td>0.532</td>
<td>0.900</td>
<td>0.743</td>
<td>0.622</td>
<td>0.821</td>
<td>0.736</td>
<td>1.146</td>
<td>1.055</td>
</tr>
<tr>
<td>H 40 MeV</td>
<td>40</td>
<td>1.50</td>
<td>1.032 ± 0.060</td>
<td>0.499</td>
<td>0.866</td>
<td>0.634</td>
<td>0.537</td>
<td>0.788</td>
<td>0.699</td>
<td>1.106</td>
<td>1.054</td>
</tr>
<tr>
<td>H 30 MeV</td>
<td>30</td>
<td>1.90</td>
<td>0.846 ± 0.022</td>
<td>0.483</td>
<td>0.849</td>
<td>0.585</td>
<td>0.497</td>
<td>0.771</td>
<td>0.680</td>
<td>1.082</td>
<td>1.047</td>
</tr>
<tr>
<td>He 150 MeV/u</td>
<td>144.2</td>
<td>2.24</td>
<td>1.027 ± 0.018</td>
<td>0.527</td>
<td>0.884</td>
<td>0.667</td>
<td>0.515</td>
<td>0.812</td>
<td>0.734</td>
<td>1.030</td>
<td>1.150</td>
</tr>
<tr>
<td>H 24 MeV</td>
<td>24</td>
<td>2.27</td>
<td>0.831 ± 0.026</td>
<td>0.470</td>
<td>0.835</td>
<td>0.552</td>
<td>0.467</td>
<td>0.758</td>
<td>0.665</td>
<td>1.061</td>
<td>1.045</td>
</tr>
<tr>
<td>H 20 MeV</td>
<td>20</td>
<td>2.64</td>
<td>0.785 ± 0.013</td>
<td>0.459</td>
<td>0.823</td>
<td>0.526</td>
<td>0.443</td>
<td>0.747</td>
<td>0.653</td>
<td>1.041</td>
<td>1.038</td>
</tr>
<tr>
<td>H 17 MeV</td>
<td>17</td>
<td>3.01</td>
<td>0.816 ± 0.019</td>
<td>0.449</td>
<td>0.811</td>
<td>0.504</td>
<td>0.423</td>
<td>0.737</td>
<td>0.642</td>
<td>1.022</td>
<td>1.038</td>
</tr>
<tr>
<td>H 14 MeV</td>
<td>14</td>
<td>3.52</td>
<td>0.752 ± 0.017</td>
<td>0.436</td>
<td>0.796</td>
<td>0.480</td>
<td>0.399</td>
<td>0.724</td>
<td>0.627</td>
<td>0.995</td>
<td>1.030</td>
</tr>
<tr>
<td>C 400 MeV/u</td>
<td>277.2</td>
<td>14.24</td>
<td>0.795 ± 0.004</td>
<td>0.496</td>
<td>0.840</td>
<td>0.502</td>
<td>0.395</td>
<td>0.757</td>
<td>0.710</td>
<td>0.511</td>
<td>0.280</td>
</tr>
<tr>
<td>C 390 MeV/u</td>
<td>384.9</td>
<td>11.17</td>
<td>0.816 ± 0.018</td>
<td>0.506</td>
<td>0.851</td>
<td>0.532</td>
<td>0.402</td>
<td>0.789</td>
<td>0.726</td>
<td>0.763</td>
<td>0.778</td>
</tr>
<tr>
<td>O 1000 MeV/u</td>
<td>444.8</td>
<td>56.80</td>
<td>0.477 ± 0.011</td>
<td>0.469</td>
<td>0.806</td>
<td>0.429</td>
<td>0.350</td>
<td>0.750</td>
<td>0.687</td>
<td>0.488</td>
<td>0.463</td>
</tr>
<tr>
<td>Ar 500 MeV/u</td>
<td>444.8</td>
<td>56.80</td>
<td>0.477 ± 0.011</td>
<td>0.469</td>
<td>0.806</td>
<td>0.429</td>
<td>0.350</td>
<td>0.750</td>
<td>0.687</td>
<td>0.488</td>
<td>0.463</td>
</tr>
<tr>
<td>Ti 1000 MeV/u</td>
<td>977.6</td>
<td>108.2</td>
<td>0.436 ± 0.012</td>
<td>0.465</td>
<td>0.807</td>
<td>0.429</td>
<td>0.364</td>
<td>0.754</td>
<td>0.703</td>
<td>0.424</td>
<td>0.354</td>
</tr>
<tr>
<td>Fe 1000 MeV/u</td>
<td>967</td>
<td>151.4</td>
<td>0.381 ± 0.029</td>
<td>0.457</td>
<td>0.798</td>
<td>0.418</td>
<td>0.359</td>
<td>0.746</td>
<td>0.695</td>
<td>0.403</td>
<td>0.346</td>
</tr>
<tr>
<td>Fe 500 MeV/u</td>
<td>423.7</td>
<td>200.3</td>
<td>0.393 ± 0.020</td>
<td>0.438</td>
<td>0.766</td>
<td>0.389</td>
<td>0.329</td>
<td>0.715</td>
<td>0.651</td>
<td>0.385</td>
<td>0.370</td>
</tr>
<tr>
<td>Fe 200 MeV/u</td>
<td>620</td>
<td>431.8</td>
<td>0.312 ± 0.006</td>
<td>0.387</td>
<td>0.697</td>
<td>0.353</td>
<td>0.282</td>
<td>0.654</td>
<td>0.562</td>
<td>0.334</td>
<td>0.447</td>
</tr>
<tr>
<td>Kr 400 MeV/u</td>
<td>313.1</td>
<td>447.2</td>
<td>0.380 ± 0.005</td>
<td>0.413</td>
<td>0.732</td>
<td>0.368</td>
<td>0.309</td>
<td>0.685</td>
<td>0.613</td>
<td>0.356</td>
<td>0.345</td>
</tr>
<tr>
<td>Xe 290 MeV/u</td>
<td>185.5</td>
<td>1368</td>
<td>0.344 ± 0.005</td>
<td>0.372</td>
<td>0.675</td>
<td>0.340</td>
<td>0.278</td>
<td>0.637</td>
<td>0.549</td>
<td>0.321</td>
<td>0.329</td>
</tr>
</tbody>
</table>
Table 8.5: Modeling of OSL $\eta_{HCP,\gamma}$ of Luxel$^\text{TM}$ detectors detecting only F-center emission band (Hoya U-340 and Schott WG-360 filters). We obtained the $\eta_{HCP,\gamma}$ values through TSM using different RDD analytical models and MC simulations with GEANT4. The $\eta_{HCP,\gamma}$ values are calculated in water.

<table>
<thead>
<tr>
<th>Beam</th>
<th>Energy (MeV/u)</th>
<th>$L_{H^2O}^\infty$ (keV/(\mu)m)</th>
<th>Experimental data</th>
<th>Chatterjee</th>
<th>Katz</th>
<th>Waligórski</th>
<th>Fageeha</th>
<th>Geiß</th>
<th>Kiefer</th>
<th>Katz-Core (This work)</th>
<th>GEANT4 (This work)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H 1000 MeV</td>
<td>1000</td>
<td>0.223</td>
<td>0.984 ± 0.185</td>
<td>0.991</td>
<td>0.892</td>
<td>0.869</td>
<td>0.707</td>
<td>0.834</td>
<td>0.786</td>
<td>0.933</td>
<td>0.897</td>
</tr>
<tr>
<td>H 230 MeV</td>
<td>230</td>
<td>0.413</td>
<td>0.936 ± 0.021</td>
<td>0.702</td>
<td>0.851</td>
<td>0.741</td>
<td>0.596</td>
<td>0.788</td>
<td>0.715</td>
<td>0.935</td>
<td>0.943</td>
</tr>
<tr>
<td>H 70 MeV</td>
<td>70</td>
<td>0.960</td>
<td>0.920 ± 0.010</td>
<td>0.493</td>
<td>0.792</td>
<td>0.573</td>
<td>0.470</td>
<td>0.732</td>
<td>0.640</td>
<td>0.907</td>
<td>0.944</td>
</tr>
<tr>
<td>H 40 MeV</td>
<td>40</td>
<td>1.50</td>
<td>0.848 ± 0.028</td>
<td>0.452</td>
<td>0.749</td>
<td>0.495</td>
<td>0.407</td>
<td>0.694</td>
<td>0.597</td>
<td>0.876</td>
<td>0.954</td>
</tr>
<tr>
<td>H 30 MeV</td>
<td>30</td>
<td>1.90</td>
<td>0.721 ± 0.022</td>
<td>0.434</td>
<td>0.727</td>
<td>0.460</td>
<td>0.377</td>
<td>0.675</td>
<td>0.574</td>
<td>0.858</td>
<td>0.954</td>
</tr>
<tr>
<td>H 24 MeV</td>
<td>24</td>
<td>2.27</td>
<td>0.710 ± 0.030</td>
<td>0.420</td>
<td>0.709</td>
<td>0.435</td>
<td>0.355</td>
<td>0.660</td>
<td>0.555</td>
<td>0.842</td>
<td>0.955</td>
</tr>
<tr>
<td>H 20 MeV</td>
<td>20</td>
<td>2.64</td>
<td>0.666 ± 0.013</td>
<td>0.408</td>
<td>0.693</td>
<td>0.415</td>
<td>0.337</td>
<td>0.647</td>
<td>0.540</td>
<td>0.827</td>
<td>0.954</td>
</tr>
<tr>
<td>H 17 MeV</td>
<td>17</td>
<td>3.01</td>
<td>0.675 ± 0.020</td>
<td>0.397</td>
<td>0.678</td>
<td>0.398</td>
<td>0.321</td>
<td>0.636</td>
<td>0.525</td>
<td>0.812</td>
<td>0.955</td>
</tr>
<tr>
<td>H 14 MeV</td>
<td>14</td>
<td>3.52</td>
<td>0.622 ± 0.022</td>
<td>0.383</td>
<td>0.659</td>
<td>0.379</td>
<td>0.302</td>
<td>0.621</td>
<td>0.507</td>
<td>0.793</td>
<td>0.955</td>
</tr>
<tr>
<td>C 400 MeV/u</td>
<td>384.9</td>
<td>11.17</td>
<td>0.684 ± 0.007</td>
<td>0.465</td>
<td>0.762</td>
<td>0.442</td>
<td>0.346</td>
<td>0.712</td>
<td>0.646</td>
<td>0.663</td>
<td>0.575</td>
</tr>
<tr>
<td>C 290 MeV/u</td>
<td>277.2</td>
<td>13.30</td>
<td>0.626 ± 0.008</td>
<td>0.454</td>
<td>0.747</td>
<td>0.420</td>
<td>0.331</td>
<td>0.698</td>
<td>0.624</td>
<td>0.635</td>
<td>0.598</td>
</tr>
<tr>
<td>O 1000 MeV/u</td>
<td>1000</td>
<td>14.24</td>
<td>0.625 ± 0.008</td>
<td>0.474</td>
<td>0.784</td>
<td>0.465</td>
<td>0.369</td>
<td>0.734</td>
<td>0.682</td>
<td>0.625</td>
<td>0.407</td>
</tr>
<tr>
<td>O 400 MeV/u</td>
<td>385.5</td>
<td>19.84</td>
<td>0.587 ± 0.029</td>
<td>0.451</td>
<td>0.745</td>
<td>0.410</td>
<td>0.328</td>
<td>0.697</td>
<td>0.630</td>
<td>0.579</td>
<td>0.499</td>
</tr>
<tr>
<td>C 135 MeV/u</td>
<td>111.2</td>
<td>24.21</td>
<td>0.489 ± 0.015</td>
<td>0.418</td>
<td>0.698</td>
<td>0.368</td>
<td>0.290</td>
<td>0.656</td>
<td>0.562</td>
<td>0.529</td>
<td>0.715</td>
</tr>
<tr>
<td>Ne 400 MeV/u</td>
<td>371.9</td>
<td>31.55</td>
<td>0.470 ± 0.016</td>
<td>0.439</td>
<td>0.730</td>
<td>0.389</td>
<td>0.316</td>
<td>0.684</td>
<td>0.615</td>
<td>0.510</td>
<td>0.463</td>
</tr>
<tr>
<td>Si 490 MeV/u</td>
<td>444.8</td>
<td>56.80</td>
<td>0.398 ± 0.009</td>
<td>0.429</td>
<td>0.718</td>
<td>0.374</td>
<td>0.310</td>
<td>0.674</td>
<td>0.608</td>
<td>0.435</td>
<td>0.371</td>
</tr>
<tr>
<td>Ar 500 MeV/u</td>
<td>450.7</td>
<td>93.34</td>
<td>0.364 ± 0.019</td>
<td>0.417</td>
<td>0.704</td>
<td>0.360</td>
<td>0.303</td>
<td>0.662</td>
<td>0.596</td>
<td>0.386</td>
<td>0.337</td>
</tr>
<tr>
<td>Ti 1000 MeV/u</td>
<td>977.6</td>
<td>108.2</td>
<td>0.313 ± 0.013</td>
<td>0.426</td>
<td>0.728</td>
<td>0.380</td>
<td>0.327</td>
<td>0.684</td>
<td>0.631</td>
<td>0.381</td>
<td>0.306</td>
</tr>
<tr>
<td>Fe 1000 MeV/u</td>
<td>967</td>
<td>151.4</td>
<td>0.315 ± 0.029</td>
<td>0.418</td>
<td>0.718</td>
<td>0.372</td>
<td>0.323</td>
<td>0.676</td>
<td>0.622</td>
<td>0.360</td>
<td>0.299</td>
</tr>
<tr>
<td>Fe 500 MeV/u</td>
<td>423.7</td>
<td>200.3</td>
<td>0.333 ± 0.020</td>
<td>0.398</td>
<td>0.678</td>
<td>0.343</td>
<td>0.290</td>
<td>0.640</td>
<td>0.571</td>
<td>0.339</td>
<td>0.309</td>
</tr>
<tr>
<td>Fe 200 MeV/u</td>
<td>120.4</td>
<td>431.8</td>
<td>0.268 ± 0.004</td>
<td>0.343</td>
<td>0.593</td>
<td>0.300</td>
<td>0.240</td>
<td>0.569</td>
<td>0.472</td>
<td>0.281</td>
<td>0.344</td>
</tr>
<tr>
<td>Kr 400 MeV/u</td>
<td>313.1</td>
<td>447.2</td>
<td>0.316 ± 0.012</td>
<td>0.372</td>
<td>0.640</td>
<td>0.322</td>
<td>0.270</td>
<td>0.607</td>
<td>0.531</td>
<td>0.307</td>
<td>0.289</td>
</tr>
<tr>
<td>Xe 290 MeV/u</td>
<td>185.5</td>
<td>1368</td>
<td>0.323 ± 0.011</td>
<td>0.329</td>
<td>0.577</td>
<td>0.291</td>
<td>0.238</td>
<td>0.555</td>
<td>0.463</td>
<td>0.270</td>
<td>0.273</td>
</tr>
</tbody>
</table>
in a large range of LET must be considered. Thus, the model and methodology presented in this section present a way to estimate $\eta_{\text{HCP,}\gamma}$ values for the particles and energies that can not be experimentally obtained.

### 8.5 RELATIVE LUMINESCENCE EFFICIENCY OBTAINED USING MONTE CARLO SIMULATIONS WITH GEANT4

This section discusses the methodology and presents the results of predictions of $\eta_{\text{HCP,}\gamma}$ using the MC code GEANT4 to calculate the RDDs (chapter 5).

To calculate the $\eta_{\text{HCP,}\gamma}$ values, eq. 8.17 was written in terms of the energy deposited. We changed the integral by a sum,

$$\eta_{\text{Al}_2\text{O}_3:C}^{\text{Al}_2\text{O}_3:C}(D_0) = \sum_i f_{\text{Al}_2\text{O}_3:C}^{\text{Al}_2\text{O}_3:C}(D_i) E_i / E_{\text{Tot}}$$  \hspace{1cm} (8.26)

where $f_{\text{Al}_2\text{O}_3:C}$ is the response function (eq. 8.19), $D_i$ and $E_i$ are the dose and energy deposited in the $i$th shell (see chapter 5), and $E_{\text{Tot}} = \sum_i E_i$ is the total energy deposited. We converted the $\eta_{\text{HCP,}\gamma}$ calculated in Al$_2$O$_3$:C obtained with GEANT4 to $\eta_{\text{HCP,}\gamma}$ calculated in water using Table 8.1. We present all the $\eta_{\text{HCP,}\gamma}$ results calculated in water.

The shape of RDD changes with the thickness $z$ of the detector. Part of this dependence we attributed to the angular dependence in the production of secondary electrons by the incident HCP. However, other factors that we could not explain are also responsible for the change in the shape of the RDD (see chapter 5). Thus, the thickness $z$ of the detectors influences the $\eta_{\text{HCP,}\gamma}$ predictions because $\eta_{\text{HCP,}\gamma}$ depends on the shape the RDD. Figure 8.9 shows the $\eta_{\text{HCP,}\gamma}$ versus $z$. For comparison, we also represent in Figure 8.9 the experimental values of the $\eta_{\text{HCP,}\gamma}$ by the dashed lines ($\pm$ one standard deviation of the data).

Figure 8.10 shows the relative luminescence efficiency calculated using RDDs sim-
Figure 8.9: Influence of the thickness $z$ of the detector on the $\eta_{HCP,\gamma}$ calculated in water using GEANT4. The dashed lines represent the interval of the experimental data for one standard deviation of the data.

Predicted with GEANT4 for three different detector’s thickness $z$. For $z = 0.01$ mm the $\eta_{HCP,\gamma}$ predictions are very poor, showing differences larger than 100 % from the experimental data (Figures 8.10a and 8.10d). For $z = 1$ mm, the predictions for low LET particles are in good agreement with experimental data (within 28 %), but strongly deviate from experimental data for high-LET particles (Figures 8.10c and 8.10f).

For $z = 0.3$ mm, which corresponds to the physical thickness of Luxel™ detectors, the predictions using GEANT4 are in overall agreement with the experimental data. Except for two beams (O 1000 MeV/u and C 135 MeV/u), the agreement between predictions and experimental data are within 35 % (Figures 8.10b and 8.10e).

Avila et al. (1996) developed a Monte Carlo code exclusive to calculate RDDs in luminescence materials. They used TSM with the RDD obtained by their code to estimate TL $\eta_{HCP,\gamma}$ of LiF for a variety of particles and energies (Avila et al., 1999; Massillon-JL et al., 2006). Although their TSM results describe the general features of $\eta_{HCP,\gamma}$ data, their ab-
Figure 8.10: Relative luminescence efficiency versus $L_\infty$ in water using RDD simulated with GEANT4 for different detector thicknesses $z$. a)-c) $\eta_{HCP,\gamma}$ when OSL from LuxelTM is detected with Hoya U-340 filter (F-center emission band). e)-f) $\eta_{HCP,\gamma}$ when OSL from LuxelTM is detected with Hoya U-340 and Schott WG-360 filters (F-center emission band).
solute values disagree for particles with $L_{\infty}^{H_2O}$ larger than 10 keV/µm (Massillon-JL et al., 2006). The disagreement reaches one order of magnitude for the predictions of $\eta_{HCP,\gamma}$ from peak 5 in LiF for a carbon beam with $L_{\infty}^{H_2O}$ of about 500 keV/µm.

Thus, we conclude that the verified agreement of about 35% between the relative luminescence efficiency determined using GEANT4 and experimental data are an improvement compared to the results reported in the literature (Avila et al., 1996; Massillon-JL et al., 2006). Not only, did the calculations include a much wider range of particles and energies, but also the overall agreement between simulations and data are much better.

The change in shape of the RDD with the thickness $z$ of the detector, which is responsible for the variation in the $\eta_{HCP,\gamma}$ needs to be further investigated. The same behavior was also observed with the FLUKA code (Mark et al., 2007).

In summary, GEANT4 demonstrated to be an useful tool for the estimation of OSL $\eta_{HCP,\gamma}$ of Luxel™ detectors. However, for more accurate $\eta_{HCP,\gamma}$ estimates, GEANT4 needs to improve the cross-section models relevant to microdosimetry, such as the SDCS for production of secondary electrons (see section 5.1). Although there are a variety of MC track structure codes that utilize more fundamental and detailed physics relevant to microdosimetry and radiobiology, all of these codes are only for calculations in water (Nikjoo et al., 2006).
CHAPTER 9

MEASUREMENT OF ABSORBED DOSE AND DOSE EQUIVALENT IN COMPLEX RADIATION FIELDS

In personnel dosimetry in space, the partial solution to the HCP dosimetry problem is to combine two or more types of detectors with complementary properties, such as TLDs and OSLDs, and plastic nuclear track detectors (PNTD) (NCRP, 2002; McKeever et al., 2007). TLDs and OSLDs are efficient for low-LET radiation ($L_{H_2O} < 10 \text{ keV/µm}$), whereas PNTDs are efficient for high-LET radiation ($L_{H_2O} > 10 \text{ keV/µm}$). Thus, the total absorbed dose can be estimated as:

$$D = D_{<10 \text{ keV/µm}}^{\text{TLD/OSLD}} + D_{>10 \text{ keV/µm}}^{\text{PNTD}} \quad (9.1)$$

where $D_{<10 \text{ keV/µm}}^{\text{TLD/OSLD}}$ is the TLD/OSLD absorbed dose for particles with $L_{H_2O} < 10 \text{ keV/µm}$, and $D_{>10 \text{ keV/µm}}^{\text{PNTD}}$ is the PNTD absorbed for particles with $L_{H_2O} > 10 \text{ keV/µm}$.

As discussed in this dissertation, the relative luminescence efficiency depends on the ionization density. The absorbed dose as-measured by TLDs/OSLDs contains contribution not only from particles with $L_{H_2O}$ lower than 10 keV/µm, but also for all the other particles that constitute the radiation field.

Fortunately, PNTD provides some information about the LET spectrum of the radiation field. Thus, knowing the $\eta_{HCP,\gamma}$ versus $L_\infty$, we can use the LET spectrum provided by PNTD to subtract the $L_{H_2O} > 10 \text{ keV/µm}$ contribution from the TLD/OSLD total absorbed...
The absorbed dose $D^{TLD/OSLD}$ (Benton et al., 2002):

$$D^{TLD/OSLD}_{<10 \text{ keV/µm}} = D^{TLD/OSLD} - \sum_{L_i=10 \text{ keV/µm}}^{1500 \text{ keV/µm}} \eta_{HCP,\gamma}^i D^{PNTD}_i$$  \hspace{1cm} (9.2)

where $\eta_{HCP,\gamma}^i$ and $D^{PNTD}_i$ are the relative luminescence efficiency, and PNTD absorbed dose from particles with LET $i$, respectively. Thus, the total absorbed dose is estimated as:

$$D = D^{TLD/OSLD}_{<10 \text{ keV/µm}} + \sum_{L_i=10 \text{ keV/µm}}^{1500 \text{ keV/µm}} D^{PNTD}_i$$ \hspace{1cm} (9.3)

Radiation protection requires not only the estimation of absorbed dose, but also the estimation of dose equivalent $H$. Using the LET spectrum provided by PNTD, $H$ is estimated as:

$$H = D^{TLD/OSLD}_{<10 \text{ keV/µm}} + \sum_{L_i=10 \text{ keV/µm}}^{1500 \text{ keV/µm}} Q_i D^{PNTD}_i$$ \hspace{1cm} (9.4)

where $Q_i$ is the quality factor for a particle with LET $i$ (ICRP, 1990), and the numerical value of $D^{TLD/OSLD}_{<10 \text{ keV/µm}}$ (in Gy) is equal to the numerical value of $H^{TLD/OSLD}_{<10 \text{ keV/µm}}$ (in Sv).

For Al$_2$O$_3$:C, TLD-100 and TLD-300, the relative luminescence efficiency is different from unity even for particles with $L_{\infty}^{H_2O}$ lower than 10 keV/µm. Thus, for reliable estimation of the absorbed dose, correction of $D^{TLD/OSLD}_{<10 \text{ keV/µm}}$ must be performed. PNTD does not provide reliable information for $L_{\infty}^{H_2O}$ lower than 10 keV/µm. Thus, methods to estimate an “effective” LET ($L_{\infty}^{eff}$) of the radiation field based on the analysis of the TL or OSL curves were developed (Yukihara and McKeever, 2006a; Yukihara et al., 2006; Gaza et al., 2006a; Berger et al., 2006; Hajek et al., 2006). For OSL from Luxel$^\text{TM}$, $L_{\infty}^{eff}$ is extracted analyzing the ratio between the OSL initial intensity and total area, providing that the shape of the OSL curve is characterized for different LETs. Using the $\eta_{HCP,\gamma}$ versus $L_{\infty}$ curve, the $L_{\infty}^{eff}$ is translated into an effective relative luminescence efficiency $\eta_{HCP,\gamma}^{eff}$ of the detector. Then,
\[ \eta_{HCP,\gamma}^{eff} \] is used to correct the TLD/OSLD absorbed dose:

\[ D_{\text{cor}}^{eff} = \frac{D_{\text{TLD/OSLD}}^{<10\text{keV}/\mu\text{m}}}{\eta_{HCP,\gamma}^{eff}} \]  \hspace{1cm} (9.5)

Figure 9.1 illustrates the determination of the \( L_{\infty}^{\text{eff}} \) and \( \eta_{HCP,\gamma}^{eff} \). This method works only for radiation fields dominated by low-LET particles.

Figure 9.1: Method to estimate the “effective” LET \( L_{\infty}^{\text{eff}} \), and effective relative luminescence efficiency \( \eta_{HCP,\gamma}^{eff} \) of the radiation field using OSL from Luxel\textsuperscript{TM}. a) Characterization of the shape of the OSL curve from Luxel\textsuperscript{TM} to different LETs. The ordinate axis represents the “Ratio” between the OSL initial intensity and total area. b) Relative luminescence efficiency as a function of LET. The OSL was measured with Hoya U-340 filters detecting F-center and UV emission bands. The red lines are arbitrary functions fitted to the data for better visualization.

Alternatively, if the particles and energies of the HCP radiation field are known, a corrected absorbed dose \( D_{\text{cor}}^{eq} \) measured by the luminescence detector is obtained by:

\[ D_{\text{cor}}^{eq} = \frac{D_{\text{TLD/OSLD}}^{<10\text{keV}/\mu\text{m}}}{\eta_{HCP,\gamma}^{eq}} \]  \hspace{1cm} (9.6)

where \( \eta_{HCP,\gamma}^{eq} \) is the equivalent relative luminescence efficiency of the detector to the radiation field the detector was exposed. \( \eta_{HCP,\gamma}^{eq} \) depends on the spectrum of charges and
energies of the particles that constitute the radiation field:

$$\eta_{HCP,\gamma}^{eq} = \sum_{Z_i, E_i} \frac{\eta_{HCP,\gamma}^i(Z_i, E_i)}{\Gamma^i(Z_i, E_i)} \quad (9.7)$$

where $\eta_{HCP,\gamma}^i(Z_i, E_i)$ is the relative luminescence efficiency for a particle with the charge $Z_i$ and energy $E_i$, and $\Gamma^i(Z_i, E_i)$ is the fraction of dose per particle with charge $Z_i$ and energy $E_i$ that constitutes the radiation field. If the spectrum of charges and energies is known, we can determine $\eta_{HCP,\gamma}^i(Z_i, E_i)$ using the TSM presented in this dissertation, or experimental data, if available. Thus, we can estimate $\eta_{HCP,\gamma}^{eq}$ and correct the absorbed dose.

The two methods presented above, $\eta_{HCP,\gamma}^{eff}$ and $\eta_{HCP,\gamma}^{eq}$, to correct the response of the detector present advantages and disadvantages. The method based on the determination of $\eta_{HCP,\gamma}^{eff}$ requires characterization of the luminescence response of the detectors as a function of LET. Thus, this method is very time consuming and expensive because HCPs relevant to radiation protection in space can be obtained only in a few accelerators located in different places worldwide. In addition, the correction factor $\eta_{HCP,\gamma}^{eff}$ presents systematic errors which are introduced when determining the “effective” LET of the radiation field.

The method based on the determination of the $\eta_{HCP,\gamma}^{eq}$ requires knowledge of the spectrum of charges and energies of the radiation field, which is complicated to accurately measure, or simulate using transport codes. In addition, inside of the ISS the spectrum of particles and energies varies with location because of different shielding composition and thickness (Benton and Benton, 2001; Benton et al., 2002). Thus, although the correction factor $\eta_{HCP,\gamma}^{eq}$ can be used to estimate the true value of the absorbed dose, the accuracy of the method depends on the accuracy of the determination of the radiation field.

We mentioned in the introduction of this dissertation that NASA is currently using Luxel<sup>TM</sup> detectors inside of the ISS to measure absorbed dose and dose equivalent (Zhou et al., 2006, 2007). However, NASA does not apply any correction to the $\eta_{HCP,\gamma}$ of the
detectors on the doses estimated by Luxel\textsuperscript{TM} detectors. Thus, the results and methodology presented in this dissertation can be used to estimate the Luxel\textsuperscript{TM} $\eta_{HCP,\gamma}^{eq}$ in different locations inside the ISS where the spectrum of charges and energies is known. Independently, the dose estimations should also be performed with the correction factor $\eta_{HCP,\gamma}^{eff}$ for cross-check and reliability. A reliable measurement of absorbed dose and dose equivalent is extremely important for the radiation protection program in space.
CHAPTER 10

CONCLUSION

This work investigated the optically stimulated luminescence (OSL) response of Luxel\textsuperscript{TM} detectors exposed to 24 combinations of heavy charged particles (HCPs) and energies relevant to radiation protection in space and cancer therapy. We used the track structure model (TSM) combined with different radial dose distribution (RDD) analytical models and Monte Carlo (MC) simulations to predict relative luminescence efficiencies, $\eta_{\text{HCP,}\gamma}$. Below we summarize the results of the experimental characterization and TSM predictions.

The OSL dose response of Luxel\textsuperscript{TM} detectors exposed to HCP beams was investigated using two different filter sets. Regardless of the filter set, we observed that beta rays and H 1000 MeV produced similar responses in the detectors, which indicated that the pattern of energy deposition by H 1000 MeV and beta rays is similar. Using Hoya U-340 filter, which detects the F-center and UV emission bands, we observed that the beta rays and H 1000 MeV caused a strong supralinearity of $f(D) = 1.8$ in the dose response curve. On the other hand, the supralinearity index for beta rays and H 1000 MeV when using a combination of Hoya U-340 and Schott WG-360 filters, which detects the F-center emission band only, was less than 1.2. Thus, we concluded that the UV emission band is responsible for most of the supralinearity in the OSL dose response of Luxel\textsuperscript{TM} detectors irradiated with beta rays and H 1000 MeV. For heavier ions from He to Fe no supralinearity was observed in the investigated range of doses for both filter sets. In the case of the Fe 200 MeV/u beam we attributed the linear-saturation behavior to the fact that high-LET particles such as Fe 200 MeV/u ions produce a pattern of energy deposition that is concentrated in regions close to the track of the particle. Thus, the luminescence saturation occurs only when the particle
fluence is high enough for the tracks to start interacting (Sawakuchi et al., 2007a).

We studied the change in shape of the OSL curves from Luxel\textsuperscript{TM} detectors for different radiation qualities and absorbed doses and observed that the important parameter that causes changes in the OSL curve is the ionization density. Beta doses of about (1-10) Gy are needed to cause changes in the OSL curves. On the other hand, for Ne 400 MeV/u and Fe 200 MeV/u radiations, the OSL curve presents further changes only for absorbed doses larger than 50 Gy. Based on the fluence corresponding to the absorbed dose of 50 Gy and analytical models of RDD, we estimated that the dose level in the inter-track region is comparable to the beta dose in which the OSL curve starts to change. This is an indication that track overlap is responsible for further changes in shape of the OSL curves of Luxel\textsuperscript{TM} detectors as the HCP fluence increases (Sawakuchi et al., 2007b).

Relative luminescence efficiency values $\eta\text{HCP,\gamma}$ of Luxel\textsuperscript{TM} detectors were determined for different detection filters to discriminate the F-center and UV emission bands. Data on OSL and TL $\eta\text{HCP,\gamma}$ of $\text{Al}_2\text{O}_3$C single crystals and TLD-100 was also obtained for comparison. A common trend of decreasing $\eta\text{HCP,\gamma}$ as increasing the LET of the radiation field was observed for all the detectors. For Luxel\textsuperscript{TM} detectors the $\eta\text{HCP,\gamma}$ is close to unit for particles with $L_{H_2O}$ lower than 3 keV/\textmu m. Then, the $\eta\text{HCP,\gamma}$ decreases and stabilizes at 200 keV/\textmu m. The $\eta\text{HCP,\gamma}$ of Luxel\textsuperscript{TM} detectors presented different values when using different detection windows to measure the OSL. We used TSM to show that this difference correlates with the luminescence response functions of the detector. These results support previous observations that the $\eta\text{HCP,\gamma}$ is ultimately characterized by the behavior of the point defects responsible for the detected luminescence signal (Yukihara et al., 2006). Using MC simulations with GEANT4, we qualitatively explained that the different values of $\eta\text{HCP,\gamma}$ for particles with the same LET, but different charges and energies are due to the different spatial pattern of energy deposition around the track of the incident particle.

The definition of $\eta\text{HCP,\gamma}$ was studied and we showed that $\eta\text{HCP,\gamma}$ has the value of unity for low LET radiation only if $\eta\text{HCP,\gamma}$ is calculated in the material of the detector and
the detector presents a “perfect” luminescence dose response (linear-saturation behavior) (Sawakuchi et al., 2007c).

We derived an expression to calculate the $\eta_{\text{HCP,}\gamma}$ based on TSM. This expression depends on the RDD and luminescence response function of the detector to low LET test radiation that mimics as closely as possible the energy spectrum of delta rays produced by the incident HCP. To calculate the $\eta_{\text{HCP,}\gamma}$, we used the following RDDs: Chatterjee and Schaefer, Butts and Katz, Waligórski et al., Fageeha et al., Kiefer and Straaten, Geiß et al. models, and MC simulations with GEANT4. In general, the analytical models failed to provide agreement better than 40%. On the other hand, the MC simulations provided agreement with experimental data within 35%.

To improve the agreement between the predicted $\eta_{\text{HCP,}\gamma}$ values and experimental data, we proposed a modified model based on Butts and Katz model, which introduces a constant region of energy deposition for small radial distances. This constant region is similar to the definition of core by Chatterjee and Schaefer, and Geiß et al. models. We determined the core region normalizing the total energy loss by path length to the LET of the particle. We proposed that the radius of the core region, which is critical when predicting $\eta_{\text{HCP,}\gamma}$, depends on properties of the incident HCP and detector. With these modifications, agreements within 15% and 20% were observed between $\eta_{\text{HCP,}\gamma}$ experimental data and modeling for the two different detection windows, respectively. This is the first time that such agreement is achieved for a wide range of particles and energies and when using a single RDD model. The model shows 20% agreement with experimental data for particles that have constant LET when passing through the detector, and with charges up to 54 and $L_{\text{c}}^{\text{H}_2\text{O}}$ up to 1368 keV/μm.

The $\eta_{\text{HCP,}\gamma}$ obtained with MC simulation presented a strong dependence on the thickness $z$ of the detector. Although we performed tests using different MC geometries, step sizes and physics models, we were unable to understand the causes of the $\eta_{\text{HCP,}\gamma}$ dependence on the thickness of the detector. Nevertheless, we verified agreement within 35%
between $\eta_{\text{HCP,}\gamma}$ experimental data and simulations if an appropriate thickness is used.

We suggested a correction method, based on the calculation of $\eta_{\text{HCP,}\gamma}$ using the TSM presented in this dissertation, to measure more reliable absorbed doses when using luminescence detectors in complex radiation fields.

To conclude this dissertation, we comment on the limitations and weakness of our model to predict the relative luminescence efficiency, suggest further improvements, and future work.

We performed two approximations in the relative luminescence efficiency formula used in the predictions. The approximations were as follows: i) we considered the factor $\eta_{\delta,\gamma}$ independent on the energy of the secondary electrons created by the incident HCP and we assumed $\eta_{\delta,\gamma}$ equal to unity; and ii) we used beta rays from a $^{90}\text{Sr}^{90}\text{Y}$ source as the test radiation. We consider these two approximations the main limitations of our approach. Thus, we encourage further investigations to accurately determine the energy response of Luxel$^\text{TM}$ detectors, which provides adequate inclusion of the energy dependent factor $\eta_{\delta,\gamma}$ in the predictions, and determination of the test radiation that best suits the energy spectrum of secondary electrons produced by the incident HCP.

The proposed RDD model, based on the introduction of a core region in the Butts and Katz RDD model, presents two free parameters. These parameters are determined fitting three values of $\eta_{\text{HCP,}\gamma}$ experimental data in a wide range of LET. Although we found a correlation between one of the free parameters with the distance between the defects responsible for the luminescence process, a definite physical meaning is still missing.

The $\eta_{\text{HCP,}\gamma}$ model presented in this dissertation is only accurate for high energy particles in which the change in LET is negligible when the particle transverses the detector. Therefore, we suggest an implementation of a numerical routine that accounts for LET changes of the particle, which is of large importance for cancer therapy dosimetry, where doses are measured in the Bragg peak.

The shape of RDDs calculated with GEANT4 depends on the detector’s thickness. We
attributed part of the dependence to the angular distribution of secondary electrons produced by the primary particle. Moreover, other factors that we could not explain cause the RDD changes. Further investigations need to be performed to better understand the RDD dependence on the detector’s thickness.

MC codes provide flexible design capabilities to reproduce experimental conditions. Therefore, we suggest testing other MC geometry setups. For example, the detector could be divided in micro voxels where the dose in each voxel is translated to signal through the luminescence response function. In this way, we can simulate the absolute luminescence dose response of the detector exposed to a HCP fluence $\Phi$. Preliminary results showed that this method reproduces the dose response of Luxel$^\text{TM}$ detectors for Fe 200 MeV/u, and also improves the agreement between $\eta_{HCP,\gamma}$ predictions and data to within 15% for particles with $Z > 2$. 
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Zajic, V. Energy vs. LET vs. range calculator version 1.24. Brookhaven National Laboratory. Software.


APPENDIX A

RELATIVE LUMINESCENCE EFFICIENCY DATA

Figures A.1, A.2, and A.3 compare the relative luminescence efficiency data from Luxel\textsuperscript{TM} detectors and OSL and TL from Al\textsubscript{2}O\textsubscript{3}:C single crystal and TLD-100 detectors. Table A.1 presents the relative luminescence efficiency data of Luxel\textsuperscript{TM} detectors that was graphically represented in section 7.3. In this table we also include OSL and TL relative luminescence efficiency of Al\textsubscript{2}O\textsubscript{3}:C single crystal and TLD-100 detectors. Section 7.3 describes the methodology used to calculate the relative luminescence efficiencies, and chapter 6 presents details about the experimental setup and OSL and TLD readouts.

![Graph](https://via.placeholder.com/150)

**Figure A.1:** $\eta_{\text{HCP,}\gamma}$ calculated in water of OSL from Al\textsubscript{2}O\textsubscript{3}:C single crystal detectors. We considered the OSL signal equal to the total area under the OSL curve. The OSL was measured with Hoya U-340 filter detecting both F-center and UV emission bands. For comparison we include the Luxel\textsuperscript{TM} data (full and dashed lines).
Figure A.2: $\eta_{HCP,\gamma}$ calculated in water of TL from $\text{Al}_2\text{O}_3$:C single crystal detectors. We considered the TL signal equal to the height of the dosimetric TL peak. The TL was measured with Corning 5-58 filter detecting both F-center emission band. For comparison we include the Luxel\textsuperscript{TM} data (full and dashed lines).

Figure A.3: $\eta_{HCP,\gamma}$ calculated in water of TL from TLD-100 detectors. We considered the TL signal equal to the height of the dosimetric TL peak. The TL was measured with Schott BG-39 filter. For comparison we include the Luxel\textsuperscript{TM} data (full and dashed lines).
Table A.1: Relative luminescence efficiency of HCP in respect to gamma radiation for 24 combinations of particles and energies. The relative luminescence efficiency was calculated in water. We considered the OSL signals from Luxel\textsuperscript{TM} and Al\textsubscript{2}O\textsubscript{3}:C single crystal detectors equal to the total area under the OSL curve, and the TL signals from Al\textsubscript{2}O\textsubscript{3}:C single crystal and TLD-100 detectors equal to the height of the dosimetric TL peaks. See section 6 for experimental details.

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<th>Beam</th>
<th>Energy (MeV/u)</th>
<th>(L_{\infty}^{H_2O}) (keV/\mu m)</th>
<th>Al\textsubscript{2}O\textsubscript{3}:C single crystal TL (5-58 or BG-39)</th>
<th>Al\textsubscript{2}O\textsubscript{3}:C single crystal OSL (U-340)</th>
<th>Luxel\textsuperscript{TM} OSL (U-340)</th>
<th>Luxel\textsuperscript{TM} OSL (WG-360 and U-340)</th>
<th>TL-100 TL (BG-39)</th>
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<td>0.998 ± 0.053</td>
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<td>0.977 ± 0.005</td>
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\textsuperscript{1}NASA Space Radiation Laboratory  
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\textsuperscript{3}Irradiations performed by Eril Research Inc.  
\textsuperscript{4}Irradiations performed by Johnson Space Center  
\textsuperscript{5}Loma Linda University Medical Center  
\textsuperscript{6}Texas A & M University  
\textsuperscript{7}Irradiations performed by Space Radiation Analysis Group, NASA
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8Irradiations performed by Oklahoma State University
<p>| | | | | | | | | | | | |
|---------|------|--------|------|--------|------|--------|------|--------|------|--------|        |
| O 400 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| HIMAC-OSU2 (2004) | 384.4 | 19.86 | 0.540 ± 0.015 | 0.503 ± 0.026 | 0.750 ± 0.032 | 0.597 ± 0.001 | 0.706 ± 0.018 |        |
| HIMAC-Eril (2005) | 385.5 | 19.84 | 0.495 ± 0.033 | 0.512 ± 0.042 | 0.769 ± 0.021 | 0.609 ± 0.013 | 0.832 ± 0.018 |        |
| HIMAC-ICB8 (2005) | 385.5 | 19.84 | 0.461 ± 0.012 | 0.526 ± 0.042 | 0.710 ± 0.023 | 0.555 ± 0.004 | 0.758 ± 0.035 |        |
| C 135 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| HIMAC-OSU1 (2004) | 111.2 | 24.41 | 0.620 ± 0.005 |        |
| HIMAC-ICB6 (2004) | 111.2 | 24.41 | 0.389 ± 0.029 | 0.626 ± 0.018 | 0.489 ± 0.015 |        |
| Ne 400 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| HIMAC-ICB4 (2003) | 368.5 | 31.70 | 0.411 ± 0.009 | 0.599 ± 0.002 |        |
| HIMAC-Eril (2005) | 372.9 | 31.51 | 0.379 ± 0.035 | 0.342 ± 0.022 | 0.560 ± 0.005 | 0.467 ± 0.016 | 0.612 ± 0.023 |        |
| HIMAC-OSU4 (2006) | 371.9 | 31.55 | 0.406 ± 0.035 | 0.382 ± 0.014 | 0.572 ± 0.004 | 0.474 ± 0.004 | 0.619 ± 0.017 |        |
| Si 490 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| HIMAC-ICB2 (2002) | 442.5 | 56.93 | 0.367 ± 0.003 | 0.326 ± 0.007 | 0.485 ± 0.004 |        |
| HIMAC-OSU4 (2006) | 444.8 | 56.80 | 0.394 ± 0.013 | 0.333 ± 0.021 | 0.469 ± 0.006 | 0.398 ± 0.009 | 0.515 ± 0.009 |        |
| Ar 500 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| HIMAC-ICB6 (2004) | 448.6 | 93.54 | 0.333 ± 0.019 | 0.452 ± 0.004 | 0.359 ± 0.019 |        |
| HIMAC-ICB8 (2005) | 450.7 | 93.34 | 0.311 ± 0.012 | 0.335 ± 0.008 | 0.441 ± 0.004 | 0.369 ± 0.007 | 0.445 ± 0.013 |        |
| Ti 1000 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| NSRL-OSU (2005) | 977.6 | 108.2 | 0.436 ± 0.012 | 0.313 ± 0.013 |        |
| Fe 1000 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| NSRL-ICB (2004) | 968.0 | 151.4 | 0.292 ± 0.055 | 0.281 ± 0.004 | 0.358 ± 0.007 | 0.285 ± 0.014 | 0.350 ± 0.011 |        |
| NSRL-Eril (2006) | 967.0 | 151.4 | 0.373 ± 0.002 | 0.317 ± 0.007 |        |
| NSRL-JSC (2006) | 967.0 | 151.4 | 0.343 ± 0.008 |        |
| Fe 500 MeV/u |  |  |  |  |  |  |  |  |  |  |        |
| HIMAC-ICB2 (2002) | 416.8 | 201.8 | 0.318 ± 0.005 | 0.297 ± 0.005 | 0.397 ± 0.003 |        |
| HIMAC-ICB4 (2003) | 416.8 | 201.8 | 0.313 ± 0.006 | 0.423 ± 0.004 |        |
| HIMAC-OSU1 (2004) | 416.8 | 201.8 | 0.394 ± 0.003 |        |
| HIMAC-Eril (2005) | 423.7 | 200.3 | 0.301 ± 0.028 | 0.282 ± 0.029 | 0.374 ± 0.018 | 0.341 ± 0.020 | 0.450 ± 0.021 |        |
| HIMAC-OSU4 (2006) | 423.7 | 200.3 | 0.344 ± 0.022 | 0.324 ± 0.030 | 0.375 ± 0.006 | 0.324 ± 0.002 | 0.437 ± 0.006 |        |</p>
<table>
<thead>
<tr>
<th>Element</th>
<th>Mass (MeV/u)</th>
<th>Energy (MeV)</th>
<th>F1 (cm⁻²/mg) ± ΔF1 (cm⁻²/mg)</th>
<th>F2 (cm⁻²/mg) ± ΔF2 (cm⁻²/mg)</th>
<th>F3 (cm⁻²/mg) ± ΔF3 (cm⁻²/mg)</th>
<th>F4 (cm⁻²/mg) ± ΔF4 (cm⁻²/mg)</th>
<th>F5 (cm⁻²/mg) ± ΔF5 (cm⁻²/mg)</th>
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<td>Fe 200 MeV/u</td>
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<td>HIMAC-ICB8 (2005)</td>
<td>124.9</td>
<td>420.6</td>
<td>0.261 ± 0.020</td>
<td>0.283 ± 0.010</td>
<td>0.341 ± 0.009</td>
<td>0.285 ± 0.009</td>
<td>0.414 ± 0.007</td>
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<td>HIMAC-OSU4 (2006)</td>
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<td>431.8</td>
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<td>0.225 ± 0.015</td>
<td>0.312 ± 0.006</td>
<td>0.268 ± 0.004</td>
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<td>Kr 400 MeV/u</td>
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<td>HIMAC-ICB6 (2004)</td>
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<td>447.2</td>
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<td>0.380 ± 0.005</td>
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<td>Xe 290 MeV/u</td>
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<tr>
<td>HIMAC-Éril (2005)</td>
<td>185.5</td>
<td>1368</td>
<td>0.252 ± 0.058</td>
<td>0.259 ± 0.043</td>
<td>0.344 ± 0.005</td>
<td>0.323 ± 0.011</td>
<td>0.392 ± 0.043</td>
</tr>
</tbody>
</table>
APPENDIX B

GEANT4 CODE FOR THE PHYSICS PROCESSES

B.1 ION PROCESSES

G4hLowEnergyIonisation* ionisation = new G4hLowEnergyIonisation();
ionisation -> SetElectronicStoppingPowerModel(particle,"ICRU_R49p");
ionisation -> SetNuclearStoppingPowerModel("ICRU_R49");
ionisation -> SetNuclearStoppingOn();
ionisation -> SetFluorescence(true);
ionisation -> ActivateAugerElectronProduction(true);
manager -> AddProcess(ionisation,-1,2,2);
manager -> AddProcess(new G4StepLimiter(),-1,-1,3);

B.2 ELECTRON PROCESSES

manager -> AddProcess(new G4MultipleScattering,-1,1,1);
manager -> AddProcess(new G4LowEnergyIonisation,-1,2,2);
G4LowEnergyBremsstrahlung* brem = new G4LowEnergyBremsstrahlung();
manager -> AddProcess(brem,-1,-1,3);
manager -> AddProcess(new G4StepLimiter(),-1,-1,3);
VITA
Gabriel Oliveira Sawakuchi
Candidate for the Degree of
Doctor of Philosophy

Dissertation: CHARACTERIZATION AND MODELING OF RELATIVE LUMINESCEENCE EFFICIENCY OF OPTICALLY STIMULATED LUMINESCEENCE DETECTORS EXPOSED TO HEAVY CHARGED PARTICLES

Major Field: Physics

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Personal Data: Born in Barretos, SP, Brazil on December 05, 1979.

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Received Bachelor of Science degree in Physics and Master of Science degree in Physics from University of Sao Paulo, Brazil, in July 2001 and in December 2003, respectively. Completed the requirements for the Doctor of Philosophy degree with major in Physics at Oklahoma State University in October 2007.

Experience:
Title of Study: CHARACTERIZATION AND MODELING OF RELATIVE LUMINESCENCE EFFICIENCY OF OPTICALLY STIMULATED LUMINESCENCE DETECTORS EXPOSED TO HEAVY CHARGED PARTICLES

Scope and Method of Study: This work investigates the optically stimulated luminescence (OSL) response of carbon-doped aluminum oxide (Al₂O₃:Ç) detectors exposed to heavy charged particles (HCPs) with energies relevant to radiation protection in space, and cancer therapy. This investigation includes ground-based experiments in accelerators and theoretical studies of the detector’s response. These theoretical studies are based on the track structure model (TSM) and require information of the spatial pattern of energy deposition around the HCP path – the radial dose distribution (RDD). Thus, RDDs were obtained using six analytical models, and Monte Carlo (MC) simulations with the code GEANT4. In addition, we propose a modified analytical model to improve the agreement between calculated and experimental efficiency values.

Findings and Conclusions: Dose response experiments showed that beta rays and H 1000 MeV radiations produced similar responses in the detectors and we concluded that the H 1000 MeV and beta radiations deposit energy similarly. We observed a common trend of decreasing the relative luminescence efficiency ($\eta_{HCP,\gamma}$) as increasing the unrestricted linear energy transfer in water ($L_{H2O}^\infty$) for all the detectors. For Luxel™ detectors the $\eta_{HCP,\gamma}$ was close to unit for particles with $L_{H2O}^\infty$ lower than 3 keV/µm. TSM using the RDD from Chatterjee and Schaefer, Butts and Katz, Waligórski et al., Fageeha et al., Kiefer and Straaten, and Geiß et al. models failed to predict the $\eta_{HCP,\gamma}$ values. We proposed a modified version of the RDD from Butts and Katz model, which agreed within 20 % with $\eta_{HCP,\gamma}$ experimental data. This was the first time that such agreement was achieved for a wide range of HCPs of different energies. MC simulations with GEANT4 agreed within 35 % with $\eta_{HCP,\gamma}$ experimental data. Finally, we suggested a correction method, based on the calculation of $\eta_{HCP,\gamma}$ using the TSM presented in this dissertation, to measure more reliable absorbed doses when using luminescence detectors in complex radiation fields.