Simulation of atom displacements induced by photons and electrons in solids

Simulatie van atoom verplaatsingen veroorzaakt door fotonen en elektronen in vaste stoffen

Proefschrift voorgelegd tot het behalen van de graad van doctor in de wetenschappen aan de Universiteit Antwerpen te verdedigen door

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“The scientist does not study nature because it is useful;

he studies it because he delights in it,

and he delights in it because it is beautiful.”

— Jules Henri Poincaré (1854–1912)
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Preface

The primary goal of radiation material science is to study the induced effects on material properties when different types of radiation pass through it. The current knowledge is comprised in the established theories which provide a description of the interaction process of those radiations with matter. Despite its explanatory success, many details still need to be fully understood and the puzzle of irradiation effects on materials is not yet complete. The primary transfer of energy is complex but well understood. The transferred energy dissipates via secondary interactions, which are not well comprehended except in a few cases.

The issue of damage caused by different radiation sources in different materials has been and is still widely discussed by the scientific community [1, 2]. This topic is of great importance involving the changes they may induce in the properties of those materials. One of the most important processes related with this radiation damage is the production of Atom Displacements (AD). There are no tools or methods for an accurate determination of AD in the case of electron and gamma radiations at present. In the late 1950’s Oen and Holmes [3] and Cahn [4] proposed a methodology to calculate the AD cross section in solids produced by gamma rays. In the last two decades several updated procedures for AD cross section estimations have been proposed. However, all those calculations have a restricted character and meaning. They follow the established calculation procedure, which does not take into account the full cascade process of the showering of gamma rays and the secondary electrons and positrons inside materials. They neither can obtain the volume distribution of damage in different positions inside the material.

Within this framework, the work presented in this thesis aims to establish a method to solve those problems and to evaluate the gamma and electron radiation damage in terms of AD. The research includes the use of mathematical modeling of physical processes taking place in irradiated materials, which lowers costs and technology needed for this type of study. Some calculation tools are also implemented in order to ease
the application of the proposed methodology. The research topic is interesting for the
development of new materials and their potential applications in several fields of research
and technology [5].

The main goals of the research are then:

1. Propose and introduce a new methodology in order to study and calculate the AD
distributions in solid materials, relating the existing theories about AD to the Monte
Carlo simulation of radiation transport in matter.

2. Compare the results obtained through the application of the proposed methodology
with previous theoretical estimations.

3. Calculate and discuss the AD distributions induced by gamma and electron irra-
diation on different technologically interesting materials applying the proposed
methodology.

The studies within this thesis are developed on the basic hypothesis that the electron-
atom elastic scattering process is fundamental in determining the formation of Atom
Displacements.

The thesis is organized in three parts. The first theoretical part gives a review of
radiation damage studies in solids and the description of the AD formation processes
within this framework. This part includes the discussion concerning cross sections for
electron scattering and incident gamma radiation. Some basic description about the
Monte Carlo method is also presented.

The second part introduces the details concerning the proposed methodology for
Monte Carlo assisted theoretical calculations of atom displacement distributions. The
implemented tools for atom displacements calculation are briefly described too. Com-
parison of some previous theoretical estimations with the results obtained through the
proposed calculation procedure is also presented and discussed.

The third part describes in detail the calculation of the displacements per atom distri-
butions in some technologically relevant materials and devices. They are the YBa$_2$Cu$_3$O$_7$
high temperature superconductor ceramic and radiation detectors for medical applica-
tions based on lutetium-yttrium oxyorthosilicate and lutetium-yttrium orthoaluminate
scintillators and on cadmium zinc telluride semiconductor.
## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preface</td>
<td>vii</td>
</tr>
<tr>
<td>1. Gamma radiation damage overview and theoretical considerations</td>
<td>1</td>
</tr>
<tr>
<td>1. General review of radiation damage in solids</td>
<td>3</td>
</tr>
<tr>
<td>1.1. Gamma irradiation effects</td>
<td>4</td>
</tr>
<tr>
<td>1.2. Radiation Damage and Atom Displacements</td>
<td>4</td>
</tr>
<tr>
<td>2. Atom Displacements: definitions and theories</td>
<td>7</td>
</tr>
<tr>
<td>2.1. Atom Displacements formation processes</td>
<td>7</td>
</tr>
<tr>
<td>2.1.1. Atom Displacements by gamma radiation</td>
<td>8</td>
</tr>
<tr>
<td>2.1.2. Atom Displacements by electrons or positrons</td>
<td>9</td>
</tr>
<tr>
<td>2.2. Threshold displacement energy</td>
<td>9</td>
</tr>
<tr>
<td>2.3. Primary knock-on atoms formation</td>
<td>11</td>
</tr>
<tr>
<td>2.4. Cross sections for electron Coulomb scattering</td>
<td>12</td>
</tr>
<tr>
<td>2.5. Cross section for incident gamma radiation</td>
<td>15</td>
</tr>
<tr>
<td>2.6. Cascades and multiple displacements</td>
<td>17</td>
</tr>
<tr>
<td>3. Monte Carlo simulation</td>
<td>19</td>
</tr>
<tr>
<td>3.1. Basic description and principles</td>
<td>19</td>
</tr>
<tr>
<td>3.2. MCNPX simulation code system</td>
<td>21</td>
</tr>
<tr>
<td>3.2.1. Photon and electron transport in MCNPX</td>
<td>21</td>
</tr>
<tr>
<td>3.3. Estimation of the Monte Carlo precision</td>
<td>23</td>
</tr>
</tbody>
</table>
## II. Developed methodology for Monte Carlo assisting theoretical calculations of atom displacement distributions

### 4. The Monte Carlo assisted Classical Method (MCCM)

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.1. MCCM description and procedure</td>
<td>27</td>
</tr>
<tr>
<td>4.2. Displacement cross section</td>
<td>30</td>
</tr>
<tr>
<td>4.3. Description of the simulation process</td>
<td>31</td>
</tr>
<tr>
<td>4.4. Working procedure for the MCCM calculations</td>
<td>32</td>
</tr>
<tr>
<td>4.5. Fluence distributions and energy deposition</td>
<td>33</td>
</tr>
<tr>
<td>4.6. Implemented calculation tools</td>
<td>35</td>
</tr>
<tr>
<td>4.6.1. MCCM functions library</td>
<td>35</td>
</tr>
<tr>
<td>4.6.2. MCCM graphical user interface</td>
<td>36</td>
</tr>
</tbody>
</table>

### 5. Comparing MCCM with the previous calculations

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1. Secondary particle fluence distribution</td>
<td>40</td>
</tr>
<tr>
<td>5.2. Dpa induced by gamma irradiation</td>
<td>42</td>
</tr>
<tr>
<td>5.3. Dpa induced by electron irradiation</td>
<td>45</td>
</tr>
<tr>
<td>5.4. Chapter conclusions</td>
<td>48</td>
</tr>
</tbody>
</table>

## III. Results calculating the displacements per atom distributions in some technologically interesting materials

### 6. Dpa distributions in YBCO superconducting material

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1. Introduction</td>
<td>54</td>
</tr>
<tr>
<td>6.2. Selection of the threshold displacement energy</td>
<td>54</td>
</tr>
<tr>
<td>6.3. Dpa in planar and chain sites under low gamma irradiation</td>
<td>56</td>
</tr>
<tr>
<td>6.3.1. Correlation between dpa and energy deposition</td>
<td>60</td>
</tr>
<tr>
<td>6.4. Dpa profiles for higher energy gamma irradiation</td>
<td>61</td>
</tr>
<tr>
<td>6.4.1. Relation between dpa and energy deposition</td>
<td>66</td>
</tr>
<tr>
<td>6.5. Study of positrons contribution to dpa profiles</td>
<td>68</td>
</tr>
<tr>
<td>6.5.1. Dpa to energy deposition ratio</td>
<td>73</td>
</tr>
<tr>
<td>6.6. Dpa profiles in YBCO irradiated with electrons</td>
<td>73</td>
</tr>
<tr>
<td>6.6.1. Displacements per atom and energy deposition</td>
<td>77</td>
</tr>
<tr>
<td>6.7. Chapter conclusions</td>
<td>78</td>
</tr>
</tbody>
</table>
7. Radiation damage evaluation on LYSO and LuYAP crystals
   7.1. Introduction .......................................................... 81
   7.2. Model for Monte Carlo simulation ............................... 84
   7.3. Threshold displacement energies ............................... 84
   7.4. Displacement cross section ..................................... 85
   7.5. Calculation of dpa distributions ............................... 85
   7.6. Displacements to energy deposition ratio ..................... 90
   7.7. Chapter conclusions ............................................. 92

8. Displacement damage by gamma rays in a CZT matrix detector
   8.1. Introduction ....................................................... 93
   8.2. System model for calculations .................................. 94
   8.3. Threshold displacement energies in CZT ....................... 95
   8.4. Displacement cross sections for CZT .......................... 96
   8.5. Determination and analysis of dpa distributions .............. 96
   8.6. Dpa to energy deposition ratio ................................ 100
   8.7. Chapter conclusions ........................................... 101

Summary ................................................................. 103

Samenvatting ............................................................ 107

Bibliography ............................................................. 111

List of figures ............................................................ 123

List of tables ............................................................ 126

Glossary ................................................................. 127

Publications related with the PhD ................................. 131

Brief Curriculum Vitae .................................................. 133
Part I.

Gamma radiation damage overview and theoretical considerations
Chapter 1.

General review of radiation damage in solids

“Elegance is the science of doing nothing like the other, seeming to do everything the same way they do.”
— Honoré de Balzac (1799–1850)

The physical properties of irradiated materials have been a subject of extensive research during the last six decades. In most of these studies, samples are exposed to an external flux of radiation such as neutrons [6–10], gammas [11–17], electrons [18–24] or ions [25–31]. The primary radiation damage is the formation of a lattice vacancy and an interstitial atom, i.e., a Frenkel pair. Over the years, significant progress has been made, experimentally and theoretically, in understanding defect production and the properties of the resulting isolated vacancies and interstitials. Several of these studies are focused on different materials and devices in radiation environments, evaluating the impact on their microscopic or macroscopic properties.

Large progress in simulating damage production and defect properties has been made over the past decade as a result of the increasing power of computational facilities [32–43]. Simulation techniques allow us to analyze several parameters and properties with lower costs and faster than in real experiments. Becquart and Domain [44] present an overview of some of the techniques used in the multiscale modeling approach of radiation damage in structural materials. This scheme resorts to different simulation techniques as many length and time scales are involved.
1.1. Gamma irradiation effects

The effects of gamma and electron radiation on materials is of great interest. The penetration distance of electrons is small, so that either inconveniently small samples must be used or inhomogeneity of damage must be allowed. The latter limitation is not present when gamma rays with energies of a few MeV are used, since their attenuation distances are larger. The advantage of gamma radiation in radiation damage studies depends mostly on its ability to introduce a homogeneous damage region throughout a large specimen. In any case it is clear that gamma rays offer a very useful tool for recent investigations in radiation damage [1, 45–52].

1.2. Radiation Damage and Atom Displacements

Irradiation of materials with particles that are sufficiently energetic to create atom displacements can induce significant microstructural alterations, ranging from the generation of large concentrations of point defects or aggregates in crystalline lattices to crystalline-to-amorphous phase transitions. These microstructural changes typically cause significant changes in the macroscopic properties of the irradiated material [53, and references therein].

In this field results relevant the determination of the induced number of displaced atoms on irradiated materials, as measure of the induced point defect density. There are no tools or methods for atom displacements accurate determination in the cases of electron and gamma radiations at present. However, it is one of the magnitudes well studied and investigated in gamma radiation damage studies in the recent years [1, 35–37, 54–57], due to its importance and interest within this field.

Previous works involving the approximate evaluation of atom displacements have been reported for high temperature superconductors and metals irradiated with electrons [19, 58, 59] and gamma rays [13, 60]. The common procedure is to evaluate the displacement cross section following the Oen and Holmes [3] and Cahn [4] proposals for electron and gamma radiations. A discussion about this topic is presented in the next chapter. However, this calculation approach does not take into account the real nature of gamma and electron interactions and transport in solids.
This gamma and electron radiation complex stochastic behavior can be very well simulated and described through calculation codes based on Monte Carlo methods, modeling the transport of different types of radiation in substance. Thus, it seems to be justified the application of this codes as an alternative way providing a more realistic approach for the gamma radiation damage calculations. An attempt introducing the Monte Carlo simulation of the atom displacement distribution induced by the gamma radiation on iron slabs has been reported by Sato et al. [61]. But at the end they calculated the number of AD by multiplying the electron track length with AD cross section, assuming an average energy of recoil atoms. However, no systematic studies concerning the application of this AD calculation approach on regard their dependence with gamma initial energy and material structural properties have not been reported.

An alternative approach to calculate the atom displacements distributions in high temperature superconductors involving gamma radiation interactions and transport properties was presented by Piñera and coworkers [35,36]. Later, the contribution from positrons was also included in these studies [37,62]. Most recently the AD distribution due to electron irradiation was investigated too [41].

Within this framework, this PhD aims to present a methodology to solve this problem, which allows studying and evaluating the gamma and electron radiation damage in different interesting materials. All this with the help of mathematical simulation of physical processes taking place in irradiated materials.
Chapter 2.

Atom Displacements: definitions and theories

“A scientist is happy, not in resting on his attainments but in the steady acquisition of fresh knowledge.”
— Max Planck (1858–1947)

The fundamental definitions and theoretical considerations concerning atom displacements processes are presented and discussed in this chapter.

2.1. Atom Displacements formation processes

The primary event begins with an energetic particle, photon, or ion, colliding with an atomic nucleus and its electron cloud. When sufficient kinetic energy is transferred to this atom, it is displaced from its crystal lattice site, leaving behind a vacancy [63]. The recoiling atom may have acquired sufficient energy to displace other atoms, and they in turn can repeat such events, leading to a collision cascade. Every displaced atom will eventually dissipate its kinetic energy and come to rest within the crystal lattice as a self-interstitial defect forming Frenkel pairs (figure 2.1). The number of Frenkel pairs created is referred to as the number of atom displacements, and their accumulated density per atom is expressed as the number of displacements per atom (dpa). Thus, when this number becomes one, then on average, each atom has been displaced once. This international standardized displacement per atom unit for radiation damage [64,65]
Atom Displacements: definitions and theories

Figure 2.1.: Formation of atom displacements when an incident particle impacts an atom from the atomic structure.

is a useful parameter for comparing displacement damage levels in a variety of radiation environments.

2.1.1. Atom Displacements by gamma radiation

The relation between masses of radiation particles and atomic species is one of the main factors influencing the efficiency in which different kind of radiation are able to transfer energy to the atoms inside irradiated material. In this sense, the gamma radiation presents the lower efficiency situation.

In this case, absorption and emission interaction mechanisms are more effective to transfer energy to atoms. In Compton scattering most of the photon energy is transferred to the scattered electrons, while the energy given to the atomic nuclei is negligible. In the absorption processes, the energy acquired by the atom in the photo-electric effect after ionization is too small compared with the photo-electron energy, and then inefficient for producing displacement. When the photon absorption takes place inside the atomic nucleus, the atom recoil energy depends on the ratio of gamma quanta energy to the nucleus rest energy. The most favorable situation is the resonant absorption of photons by the atomic nuclei, as happens through the Mössbauer effect [66]. But this effect has
only been observed in a limited number of atomic nuclei and for specific characteristic energies. Still, in those cases the atom recoil energies are in the range up to about 0.1 eV, also insufficient to be displaced.

In conclusion it is clear that the gamma radiation itself is not able to efficiently transfer enough energy in order to produce atom displacements. The secondary electrons and positrons are then the basic responsible for this process.

2.1.2. Atom Displacements by electrons or positrons

The interaction processes of electrons (or positrons) with atoms could be separated in two categories: (a) inelastic scattering processes involving both the electron-electron interactions (secondary electrons are scattered by atom electronic cloud) and the bremsstrahlung (braking radiation) process by which an electron looses energy by radiating photons; and (b) atomic elastic scattering processes (part of the electron momentum and energy is directly transferred to the atom).

All these processes have been well studied by several authors [63,67–72]. In case (a) the recoil energy received by the atomic nuclei - electronic cloud system is too small and then insufficient to provoke atom displacements, and the same occurs by bremsstrahlung processes. Therefore, atom displacements take place predominantly through the atomic elastic scattering processes. The recoil energy of atoms in this case depends on the electron to atomic mass ratio as well as on the electron scattering angle.

2.2. Threshold displacement energy

One of the basic quantities defining the radiation hardness of a material is the threshold displacement energy, $T_d$, defined as the energy needed to displace an atom in order to create a stable Frenkel pair. The concept of threshold displacement energy was probably devised by Wigner in the early 1940’s, as reported by Burton [73]. Already in 1949 it appeared as a functional parameter in Seitz’s model to treat elastic collisions [63], where it was assessed as equal to the cohesive energy plus the formation energy of the Frenkel pair (in total about 25 eV). Since then it has played a key role in radiation damage theory.
The displacement energy is difficult to measure experimentally. One way to measure this in metals is by employing an electron beam to produce the radiation damage in a thin film and monitoring its rise in electrical resistivity due to the produced defects. By reducing the energy of the electron beam, the resistivity rise is also reduced, and a threshold electron energy, $E_c$, can be found below which no displacements are produced. The corresponding recoil energy is given by relativistic kinematics as:

$$T_d = \Lambda E_c \left( \frac{2mc^2 + E_c}{2mc^2 + E_c} \right) = 4mE_c \left( 1 + \frac{E_c}{2mc^2} \right) \approx 4mME_c \left( 1 + \frac{E_c}{2mc^2} \right)$$

(2.1)

where $mc^2$ is the electron rest energy and $\Lambda = 4mM/(m + M)^2$. The approximation on the right is adequate because the electron mass, $m$, is much smaller than the recoiling atom mass, $M$.

It has been observed that the threshold energy varies significantly by changing the electron beam direction in relation to the single crystal film sample orientation. However, for polycrystalline samples, an averaged value over all orientations is obtained.

A trend that $T_d$ increases with the melting temperature has been observed in metals, reflecting the fact that larger bond strengths or cohesion energies between atoms also lead to higher melting temperatures [74, 75]. Wolfer [75] also showed that the displacement energy required to create a Frenkel pair is much larger than the combined formation energies of the vacancy and the self-interstitial. There exist a large energy barrier to create the Frenkel pair, namely the displacement energy $T_d$, and this barrier is mainly associated with the insertion of the interstitial into the crystal lattice.

Obtaining the displacement energy experimentally in compounds and non-conductor materials is more difficult, since several atomic species are involved and previously described measurements are not possible. The easiest practical procedure in this case is to follow Seitz [63] who takes an isotropic value of 25 eV, and modifying this value only when experimental values are available. This procedure has generally been applied in previous works. Zinkle and Kinoshita [76] reviewed the available information on several key parameters that describe defect production and migration in irradiated ceramics. Specifically, their review focused on the experimental and calculated values of threshold displacement energies for several technologically important oxide and carbide ceramics.

Molecular dynamics (MD) [77, 78] is well known to be a suitable simulation tool for the study of displacement cascades and the analysis of the mechanisms of formation and motion of interstitial atoms and their clusters [79–81]. The availability of MD to
evaluate $T_d$ has been demonstrated and then the MD technique has been widely used to study threshold displacement energies in several materials [82–86]. Nordlund and coworkers [85] provided a comparison of threshold behavior obtained through MD with different interatomic potentials and approximations in iron and discussed several different possible definitions of the threshold displacement energy.

2.3. Primary knock-on atoms formation

The first step in producing radiation effects is the generation of a primary recoil atom (PKA = primary knock-on atom). Such events take place very rapidly, typically occurring in much less than 1 fs ($10^{-15}$ s). The PKA dissipates its initial kinetic energy in two ways: some energy is lost by exciting the medium or PKA electrons; such excitations may lead to ionization of some particles. The PKA causes nearly elastic collisions with target atoms: the total atomic kinetic energy is nearly conserved. Because the individual electron excitation energies are small and especially because of the small momentum carried by electrons, they can be ignored in collision dynamics. Such events are said to be quasielastic. The important role of PKA spectra have been recently reviewed by Zinkle [53].

As stated above for any given incident radiation type there is an interaction with lattice atoms by which kinetic energy is transferred to the atom from the radiation. Let us suppose that this interaction can be described through a differential cross section $d\sigma(E,T)/dT$. Then for a radiation fluence, $\Phi(E)$, the density of atoms receiving a transferred energy $T$ in the interval $dT$ will be:

$$N_a \frac{d\sigma(E,T)}{dT} \Phi(E)dT \quad 0 \leq T \leq T_{\text{max}}(E)$$

with $N_a$ being the number of atoms per unit volume.

Then, the total number of primaries per unit volume is:

$$N_T = N_a \int_{T_d}^{T_{\text{max}}} \int_{E_c}^{E_{\text{max}}} \frac{d\sigma(E,T)}{dT} \Phi(E) dE,$$

where $T_d$ is the minimum energy an atom needs to be displaced, $E_c$ is the lowest radiation energy which can transfer energy $T_d$ to a lattice atom and $E_{\text{max}}$ is the maximum energy
of the radiation spectrum. Thus, for a monoenergetic incident fluence, it is possible to evaluate the total number of primaries per unit volume as:

\[ N_T = N_a \cdot \sigma(E_0) \cdot \Phi_0, \]  

being \( E_0 \) the energy of the incident radiation fluence \( \Phi_0 \). Here, the cross section \( \sigma(E_0) \) could be seen as the probability that an incident particle with energy \( E_0 \) produces a primary in the material unit volume. Therefore, the point is to find the adequate cross section for each case under study.

This thesis involves the study of radiation damage induced by gamma and electron incident radiations, which are then analyzed in the following sections. Analysis about other type of incident radiation can be found for example in [87].

2.4. Cross sections for electron Coulomb scattering

The penetration of atomic particles through matter has been the subject of considerable study, both theoretical and experimental, since the beginning of the last century. Thompson [88] first discussed the slowing down of energetic particles in matter as a result of collisions with the electrons in the atoms of the material. Five years later Rutherford [89], by studying \( \alpha \)-particle scattering, discovered the atomic nucleus and demonstrated the validity of the Rutherford formula for scattering of charged particles by a Coulomb field. Shortly thereafter Bohr [90,91] worked out the classical theory of stopping power. Later, the development of the quantum theory was responsible for considerably more work on the scattering and stopping of high-energy atomic particles in matter.

As discussed before, the production of atom displacements by electrons is dominated by the elastic scattering with atoms. At the root of all elastic scattering processes involving charged particles lies Rutherford’s famous formula [89]:

\[ \frac{d\sigma}{d\Omega}(\theta, E) = \left( \frac{Ze^2}{16E^2} \right)^2 \csc^4(\theta/2). \]  

This formula expresses the differential cross section for scattering incident particles of kinetic energy \( E \) against static charged point centers, such as heavy nuclei (charge \( Ze \)), \( \theta \) is the particle scattering angle and \( d\Omega(= 2\pi \sin \theta d\theta) \) is the solid angle for an annular cone of width \( d\theta \) about \( \theta \).
While the Rutherford scattering law applies to medium energy particles, it is not a relativistic formula and does not take into account the possible spins or identity of the scattering partners. The relativistic expression for the classical electron scattering was given by Darwin [92]:

$$\frac{d\sigma_{RD}}{d\Omega}(\theta, E) = \left(\frac{Ze^2}{2mc^2}\right)^2 \frac{1 - \beta^2}{\beta^4} \csc^4(\theta/2), \quad (2.6)$$

where $m$ is the rest mass of the electron and $\beta = v/c$ is the electron to light velocity ratio.

Mott considered relativistic scattering of Dirac particles, such as electrons, against point nuclei [93, 94], following a quantum mechanical description. In this case, the electron is assumed to have a spin (and a Dirac magnetic moment). The cross section has been expressed by Mott in terms of two conditionally convergent infinite series, which are defined by Legendre expansion. His formula is rigorously correct but is sufficiently unwieldy to have provided the incentive for the development of approximate expressions. It is common practice to express the cross section as a numerical factor, $R$, times the Rutherford-Darwin cross section:

$$\frac{d\sigma}{d\Omega}(\theta, E) = R \cdot \frac{d\sigma_{RD}}{d\Omega}(\theta, E). \quad (2.7)$$

This factor depends on $Z$, $\beta$ and $\theta$. The general form of $R$ is to approach unity from above for small scattering angles and to decrease below unity for large scattering angles; hence low-energy transfers are enhanced relative to the classical description.

Mott derived an approximate formula (the “Mott formula”) [94] which is valid for high relativistic electrons ($\beta \approx 1$) and when $\alpha/\beta \ll 1$ (light elements), where $\alpha$ equals:

$$\alpha = \frac{Ze^2}{\hbar c} \approx \frac{Z}{137}. \quad (2.8)$$

However, for more massive nuclei, where $Z$ is large, Mott’s approximation has been shown to fail, as expected.

McKinley and Feshbach have expanded Mott’s series in a power series in $\alpha$ and $\alpha/\beta$ [95]. They obtained an analytical expression for the $\alpha^2$ approximation, verified by Dalitz [96] following the second Born approximation:

$$R_{MCF} = 1 - \beta^2 \sin^2(\theta/2) + \pi \alpha \beta \sin(\theta/2) \left[1 - \sin(\theta/2)\right]. \quad (2.9)$$
This approximation is valid up to middle $Z$ elements, giving results accurate to $1\%$ for nuclei up to about $Z=40$ for high scattering angles. A closed formula, similar to (2.9) cannot be given for all values of $Z$, but numerical evaluation of the scattering for high $Z$ is given by Feshbach [97].

McKinley and Feshbach expansion have been extended by Curr [98] in order to be applicable for higher $Z$. The results have been further simplified by putting them in the form of a single power series:

$$R_c(\beta) = R(1) + (1 - \beta^2)\Delta R,$$

where $R(1)$ ($R_c$ for $\beta=1$) and $\Delta R$ are independent of energy. Curr gave these parameters as a power series in $\alpha$. The first-order terms in $\alpha$ give the McKinley and Feshbach expression. The Curr series give results accurate to $1\%$ for $\alpha/\beta$ less than 0.6 ($Z \sim 82$).

As a validity check, Curr compared his numerical results with Yadav's [99] calculations for Uranium ($\alpha=0.672$), which used Mott's exact series. Curr showed a comparison of Yadav's results at $E=20mc^2$ with the $\alpha^8$ approximation of his series, together with the results obtained by the McKinley and Feshbach and Curr $\alpha^5$ approximation (figure 2.2, taken from [98]). As can be seen, the quantum mechanical results have fewer large electron scattering angle events (fewer high energy recoil atom events) than the Rutherford-Darwin expression and vice versa for the intermediate angle (energy) events.

![Figure 2.2.](image_url)  
**Figure 2.2.** Values for the ratio of the scattering to Rutherford-Darwin cross section for the Curr $\alpha^8$ approximation and the exact calculation of Yadav for Uranium at $20mc^2$ electron energy. The McKinley and Feshbach and Curr $\alpha^5$ approximations are also shown [98].
Also, the McKinley and Feshbach approximation is quite acceptable for low and high scattering angles, in spite of the high $Z$ value.

2.5. Cross section for incident gamma radiation

Gamma radiation produces atom displacements mainly through secondary electrons and positrons. The calculation of the differential cross section is thus complex, since it involves different intermediate processes. Each of these processes may be dominant for a given energy and a given target material. Oen and Holmes [3] proposed a methodology to calculate displacement cross sections in solids by gamma rays. Cahn [4] also applied this methodology to calculate the total number of displaced atoms in germanium and silicon due to electrons and gamma rays of energies up to 7 MeV.

Following their idea, the true cross section in this case may be expressed formally by:

$$
\frac{d\sigma(E_\gamma, E)}{dE} = \sum_i \frac{d\sigma^i(E_\gamma, E)}{dE},
$$

where the index $i$ refers to the various mechanisms for energy transfer from primary gamma radiation, with energy $E_\gamma$, to secondary electrons, with kinetic energy $E$. In general, the calculated energy dependence obtained for the secondary electrons spectrum will depend upon how many processes have been included.

For these processes, the intermediate electron behavior details in the lattice must be considered. Since one of the principal experimental advantages of gamma rays is near uniformity of damage production over large samples it is felt that the most useful calculation considers the entire range of the electron as falling within the specimen. Thus, one additional result is the “thick target” cross sections for atom displacement by electrons. Then the desired cross section is:

$$
\sigma(E_\gamma) = \sum_{i=1}^{n} \int_{0}^{\infty} \frac{d\sigma^i(E_\gamma, E_0)}{dE_0} \bar{\pi}(E_0) dE_0, \tag{2.12}
$$

where $\bar{\pi}(E_0)$ is the average number of displaced atoms produced over the range of an electron with initial energy $E_0$.

It is assumed therefore that the energetic electrons produced by the gamma rays are stopped inside the solid sample. The average number, $\bar{\pi}(E_0)$, is thus found by integrating
the elastic electron-atom interaction cross section over the range of the electron, also known as the displacements cross section $\sigma_d(E)$:

$$\bar{n}(E_0) = \int_0^{X_0} N_a \sigma_d(E(x)) \, dx = N_a \int_0^{E_0} \frac{\sigma_d(E)}{(-dE/dx)} \, dE,$$  \hspace{1cm} (2.13)

where $X_0$ is the electron effective range and $(-dE/dx)$ is the stopping power which represents the electron energy change with respect to the electron path [100]. The electron-atom interaction cross section was discussed in details in the previous section.

For the $d\sigma^i(E_\gamma, E_0)$ cross sections, Oen and Holmes considered Compton scattering with the assumption of single displacement for the PKA energy higher than the displacement energy. Cahn considers the main three processes of gamma interaction with matter producing secondary electrons: Compton scattering, photoeffect and pair production. In the last two decades several updated cross sections have been proposed. The calculation by Baumann [101] was based on Oen’s electron-induced displacement cross section with the displacement energy of 28 eV and 40 eV [102], considering Compton scattering and pair production. Alexander and Rehn [103] carried out their calculation considering all three gamma-material interactions with the McKinley-Feshbach approximation for electron-induced displacement. Kwon and Motta [104] proposed dpa cross sections for various metals, considering three gamma-material interactions and using Oen’s electron-induced displacement cross section with the displacement energy of 24 eV and 40 eV. The contribution of positrons produced from the pair production was neglected in Kwon-Motta’s calculation and was treated as electrons’s in Baumann’s and Alexander-Rehn’s calculations. Fukuya and Kimura [54] calculated gamma-induced dpa cross sections of iron considering all three gamma-material interactions with the McKinley-Feshbach approximation for electron-induced displacement and displacement energies of 25 eV and 40 eV. They separately accounted for both electron and positron-induced displacements.

All these calculations have a restricted character. They follow the standard calculation procedure, which does not take into account the cascade process of the showering of gamma rays and the secondary electron and positron, occurring during radiation transport inside materials. They neither can obtain the volume distribution of dpa damage inside the material. The proposal of this thesis is to improve all these evaluations.
2.6. Cascades and multiple displacements

Beginning with the work of Brinkman \cite{70,105}, various models were proposed to compute the total number of atoms displaced by a given PKA as a function of energy. However, the Kinchin and Pease model \cite{106} was the most widely cited. This model follows from the assumptions of hard sphere isotropic scattering, an amorphous solid, a well-defined displacement threshold and no kinetic energy lost in the displacement process. For primary energies between $T_d$ and $2T_d$, the moving atom may be captured by a vacancy site left by another struck atom without causing additional displacements. Their model assumed that between a specified threshold energy and an upper energy cut-off, there was a linear relation between the produced number of Frenkel pair and the PKA energy. Above the upper energy cut-off, it was assumed that the additional energy was dissipated in electronic excitation and ionization, as it happens for ion energies higher than the Bragg peak threshold energy. The damage function $\nu(T)$ is then introduced to describe the probability that a primary atom provokes further displacements:

$$\nu(T) = \begin{cases} 1, & T_d \leq T \leq 2T_d; \\ \frac{T}{2T_d}, & T \geq 2T_d; \end{cases} \tag{2.14}$$

Later, Lindhard and coworkers developed a detailed theory for energy partitioning that could be used to compute the fraction of the PKA energy that was dissipated in the nuclear system in elastic collisions and in electronic losses \cite{107}. Nelson \cite{108} proposed a semi-empirical modification of the Kinchin-Pease model incorporating a number of important corrections. Torrens and Robinson \cite{109,110} have constructed computer simulations of collision cascades in which the trajectories of displaced atoms in a crystalline solid are followed through a sequence of isolated binary collisions. They propose a modified Kinchin-Pease model introducing the total energy lost in the cascade by electron excitation and the damage energy. Binary collision simulations using the vacancy capture model and cascade simulation by molecular dynamics have been also performed to study this phenomenon \cite{38,110–115}. Because of the high computation time required, only small crystals can be studied and the PKA energy cannot exceed approximately 1 keV. Also, extensive statistical analysis of results is difficult. Norgett, Robinson and Torrens (NRT) develop a secondary displacement model that is still used as a standard in the nuclear industry and elsewhere to compute atomic displacement rates \cite{64}. Their
model uses the modified Kynch-Pease formula of Torrens and Robinson and the inelastic energy loss calculated according to the method of Lindhard and coworkers.

For a deeper understanding about this topic, a good reference is the work of Robinson [116], where the concepts of elementary cascade theory as a basis for intuitive descriptions of the damage process were presented.
Chapter 3.

Monte Carlo simulation

“An investment in knowledge pays the best interest.”
— Benjamin Franklin (1706–1790)

Basic description and principles of the Monte Carlo method applied to simulation of radiation transport are briefly presented in this chapter. Some main characteristics of the simulation code used here are summarized as well.

3.1. Basic description and principles

The name “Monte Carlo” was coined in the 1940’s by scientists working on the nuclear weapon project in Los Alamos to designate a class of numerical methods based on the use of random numbers. Nowadays, Monte Carlo methods are widely used to solve complex physical and mathematical problems [117–119], particularly those involving multiple independent variables where more conventional numerical methods would demand formidable amounts of memory and computer time. The book by Kalos and Whitlock [119] gives a readable survey of Monte Carlo techniques, including simple applications in radiation transport, statistical physics, and many-body quantum theory. Also, Shultis and Faw [120] bring a very detailed description of the Monte Carlo method applied to radiation transport.

In Monte Carlo simulation of gamma radiation transport, the history (track) of a particle is viewed as a random sequence of free flights that end with an interaction event where the particle changes its direction of movement, loses energy and, occasionally,
produces secondary particles. The Monte Carlo simulation of a given experimental arrangement consists on the numerical generation of random histories. An “interaction model” is needed to simulate these histories, i.e., a set of differential cross sections (DCS) for the relevant interaction mechanisms. The DCSs determine the probability distribution functions (PDF) of the random variables that characterize a track: 1) free or quasi-free path between successive interaction events, 2) type of interaction and 3) energy loss and angular deflection in a particular event (and initial state of emitted secondary particles, if any). Once these PDFs are known, random histories can be generated by using appropriated sampling methods. If the number of generated histories is large enough, quantitative information on the transport process may be obtained by simply averaging over the simulated histories.

The Monte Carlo method yields the same information as the solution of the Boltzmann transport equation, with the same interaction model, but is easier to implement [121], specially for the solution of problems with complex boundary geometries. In particular, the simulation of radiation transport in infinite samples is straightforward, while even the simplest finite geometries (e.g., thin foils) are very difficult to be dealt with by the transport equation. The main drawback of the Monte Carlo method lies in its random nature: all the results are affected by statistical uncertainties, which can be reduced at the expense of increasing the sampled population and, hence, the computation time. Under special circumstances, the statistical uncertainties may be lowered by using variance-reduction techniques [122,123].

The time required to perform a particular calculation depends upon the model complexity, the details or resolution used to model the particle tracks, the required precision of the final result, and the computer speed for complex floating-point operations. Computers available now are significantly faster than supercomputers from the 1980’s and early 1990’s, so calculations giving useful results can be obtained in only a few hours (or even minutes, if using a Grid-based system).

Several Monte Carlo codes are currently available for transport simulation, i.e., ETRAN [124,125], ITS3 [126,127], EGS4 [128], EGSnrc [129], PENEOPE [130,131], GEANT-4 [132], MCNP [133,134], MCNPX [135], FLUKA [136]. All these codes are widely used within their principal application areas. Some codes require significant programming knowledge, but some do not. Some codes allow you to manage the physics involved, while with others the physics is already incorporated and close to changes. Some reviews of Monte Carlo codes are available [137], discussing their similarities and
differences, their pros and cons. The MCNPX is used for the simulations performed within our studies, since it gives the desire results in a convenient format.

3.2. MCNPX simulation code system

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. Specific areas of application include, but are not limited to, radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, nuclear oil well logging, accelerator target design, fission and fusion reactor design, decontamination and decommissioning.

MCNPX stands for Monte Carlo N-Particle eXtended. It extends the capabilities of MCNP to nearly all particles, nearly all energies, and to nearly all applications without an additional computational time penalty. MCNPX is fully three-dimensional and time dependent. It utilizes the latest nuclear cross section libraries and uses physics models for particle types and energies where tabular data are not available.

Detailed information about this code can be found elsewhere [135] (http://mcnpx.lanl.gov/documents.html). Some items related to photon and electron transport will be discussed in the next section because of their importance for the studies concerning this thesis.

3.2.1. Photon and electron transport in MCNPX

MCNPX has two photon interaction models: simple and detailed.

The simple physics treatment ignores coherent (Thomson) scattering and fluorescent photons from photoelectric absorption. It is intended for high-energy photon problems or problems where electrons are considered free.

The detailed physics treatment includes coherent scattering and accounts for fluorescent photons after photoelectric absorption. Form factors are used to account for electron binding effects. Analog capture is always used. It is the best treatment for most applications, particularly for high Z nuclides or deep penetration problems. The detailed physics treatment is used in all simulations carried out in our studies.
The generation of electrons from photons is handled in three ways. These three ways are the same for both the simple and detailed photon physics treatments. (1) If electron transport is turned on, then all photon collisions except coherent scatter can create electrons that are banked for later transport. This is the case used in our simulations. (2) If electron transport is turned off, then a thick-target bremsstrahlung model (TTB) is used. This model generates electrons, but assumes that they travel in the direction of the incident photon and that they are immediately annihilated. Any bremsstrahlung photons produced by the nontransported electrons are then banked for later transport. Thus electron-induced photons are not neglected, but the expensive electron transport step is omitted. (3) If indicated by the user in the input file, then all electron production is turned off, no electron-induced photons are created, and all electron energy is assumed to be locally deposited.

The transport of electrons and positrons is fundamentally different from that of photons. The interaction of neutral particles is characterized by relatively infrequent isolated collisions, with simple free flight between collisions. By contrast, the transport of electrons/positrons is dominated by the long-range Coulomb force, resulting in large numbers of interactions with small energy transfer.

Considerable theoretical work has been done to develop a variety of analytic and semi-analytic multiple-scattering theories for the transport of charged particles. These theories attempt to use the fundamental cross sections and the statistical nature of the transport process to predict probability distributions for significant quantities, such as energy loss and angular deflection. The most important of these theories for the algorithms in MCNPX are the Goudsmit-Saunderson [138] theory for angular deflections, the Landau [139] theory of energy-loss fluctuations, and the Blunck-Leisegang [140] enhancements of the Landau theory. These theories rely on a variety of approximations restricting their applicability, so that they cannot solve the entire transport problem. In particular, it is assumed that the energy loss is small compared to the kinetic energy of the electron.

In order to follow an electron through a significant energy loss, it is necessary to break the electron’s path into many steps. These steps are chosen to be long enough to encompass many collisions (so that multiple-scattering theories are valid) but short enough that the mean energy loss in any one step is small (so that the approximations necessary for the multiple-scattering theories are satisfied). The energy loss and angular deflection of the electron during each of the steps can then be sampled from probability distributions based on the appropriate multiple-scattering theories. This assumption
of the effects of many individual collisions into single steps that are probabilistically sampled constitutes the “condensed history” Monte Carlo method [121].

3.3. Estimation of the Monte Carlo precision

MCNPX results are normalized to be per starting particle and are printed in the output accompanied by a second number $r$, which is the estimated relative error defined to be one estimated standard deviation of the mean divided by the estimated mean, $SD(\bar{x})/\bar{x}$. In MCNPX, the quantities required for this error estimate are computed after each complete Monte Carlo history, which accounts for the fact that the various contributions to a result from the same history are correlated. For a well-behaved result, $r$ will be proportional to the inverse of the number of histories square root.

The estimated relative error can be used to form confidence intervals about the estimated mean, allowing one to make a statement about what the true result is. The Central Limit Theorem states that as the number of histories approaches infinity there is a 68% chance that the true result will be in the range $\bar{x}(1 \pm r)$ and a 95% chance in the range $\bar{x}(1 \pm 2r)$. It is extremely important to note that these confidence statements refer only to the precision of the Monte Carlo calculation itself and not to the accuracy of the result compared to the true physical value. A statement regarding accuracy requires a detailed analysis of the uncertainties in the physical data, modeling, sampling techniques, and approximations, etc., used in a calculation.

The quantity $r$ should be less than 0.10 to produce generally reliable confidence intervals. The estimated uncertainty in the Monte Carlo result must be presented with it so that all are aware of the estimated precision of the results.
Part II.

Developed methodology for Monte Carlo assisting theoretical calculations of atom displacement distributions
Chapter 4.

The Monte Carlo assisted Classical Method (MCCM)

“Imagination is more important than knowledge”
— Albert Einstein (1879–1955)

4.1. MCCM description and procedure

The proposed Monte Carlo assisted Classical Method (MCCM) relates the Oen-Holmes and Cahn established theories [3, 4] (here on referred as “classical theories”) about atom displacements to the electron and positron fluence distributions calculated from the Monte Carlo simulation.

The proposal mainly consists in replacing the analytical distributions of particles produced in gamma and electron interactions with material (expressions (2.12) and (2.13)) by those obtained through the Monte Carlo simulation of radiation transport in matter. That is, defining the total number of atom displacements (AD) per unit volume as:

\[
N_{\text{AD}} = \frac{1}{V} \int_0^{E_0} \pi(E) \cdot N_e(E) \, dE,
\]

(4.1)

where \(V\) is the studied volume, \(\pi(E)\) is the number of displaced atoms produced by an electron/positron over its path (given by (2.13)), and \(N_e(E)\) is the energy distribution of
secondary particles calculated by Monte Carlo simulation in the volume $V$. The MCNPX code system is used for simulation purposes in the studies presented here. MCNPX allows to obtain the energy fluence distribution, $\Phi_e(E)$, in the volume of the studied material. In order to study the in-depth and volumetric dpa distributions, it is possible to divide the volume of the material in subvolumes (voxels). This way the energy fluence distribution in each one of these voxels, $\Phi_e(E, z)$, can be obtained. Thus, the energy distribution of secondary particles can be computed as $\Phi_e(E) \cdot S$, being $S$ the total section of the material (or voxel) surrounding the volume $V$. This is more realistic than simply taking the theoretical distributions of secondary electrons produced in gamma-material interaction processes, as has been done so far.

As stated in Chapter 2, the displacement of an atom occurs for particle energies higher than a cutoff energy $E_c$. Then, after making some transformation (4.1) can be rewritten as:

$$N_{AD} = N_a \int_{E_c}^{E_0} \sigma_d^s(E) \cdot \Phi_e(E) \, dE,$$

(4.2)

with

$$\sigma_d^s(E) = \frac{S}{V} \int_{E_c}^{E} \frac{\sigma_d(E')}{-dE'/dx} \, dE',$$

(4.3)

where the displacement cross section, $\sigma_d(E)$, will be discussed in the next section.

All the simulation results in MCNPX are obtained normalized per incident photon or particle source. Thus, knowing the source fluence used in specific study, it is possible to obtain the total number of AD:

$$N_{AD} = N_a \Phi_0 S \int_{E_c}^{E_0} \sigma_d^s(E) \cdot \Phi_e(E) \, dE.$$

(4.4)

A more common used way of expressing atom displacements is by computing the displacements per atom magnitude, which could be obtained normalizing to the total number of atoms, $N_{AD}/N_a$. Furthermore, for compound materials all the constituent atomic species could be considered taking into account the relative fraction $n_k$ of the $k$-atom in its crystalline sublattice. Thus the total displacements per atom can be
calculated as the sum over all the atomic species:

\[ N_{dpa} = \sum_k n_k \Phi_0 S \int_{E^k_{c}}^{E_0} \sigma^k_{dpa}(E) \cdot \Phi_e(E) \, dE \].

(4.5)

The electron or positron cutoff kinetic energy depends on the \( k \)-atom mass, \( M_k \), and displacement energy, \( T^k_d \), from (2.1):

\[ E^k_c = \sqrt{(mc^2)^2 + \frac{M_k c^2}{2} T^k_d - mc^2}. \]

(4.6)

Expression (4.5) can be rewritten in the form of (2.4):

\[ N^k_{dpa} = \Phi_0 \cdot \sigma^k_{dpa}(E_0, T^k_d), \]

(4.7)

by defining the effective dpa cross section for the \( k \)-atom, depending on the incident radiation energy and the displacement energy, as follows:

\[ \sigma^k_{dpa}(E_0, T^k_d) = n_k S \int_{E^k_{c}}^{E_0} \sigma^*_{d}(E) \cdot \Phi_e(E) \, dE. \]

(4.8)

In this way, the MCCM constitutes a substantial improvement to the Oen-Holmes and Cahn algorithms, and it is not a simple quiddity. It adapts these algorithms to the modern calculations of the gamma and electron radiation transport through Monte Carlo method. In this case the approximate expressions taken \emph{a priori} for the electron energy distributions in their primary interactions are not used, like it was made, for example, by Belevtsev \textit{et al.} [13]. Full comparisons between MCCM and classical estimations are presented and discussed in the next Chapter 5.

The fact of introducing \( \Phi_e(E) \) allows to take into account more realistic electron and positron energetic distributions in any point of the solid matrix. In addition, it is possible to obtained for the first time the in-depth dpa distribution profiles subdividing the material volume in voxels. MCCM procedure also permits to evaluate more accurately the contribution to dpa from different crystalline sublattices depending on the incident gamma or electron radiation.
4.2. Displacement cross section

The different physical assumptions mentioned in previous chapter result in differences in the size and energy dependence of the displacement cross section.

In order to get an analytical expression, the $\alpha^2$ approximation of McKinley and Feshbach (2.9) is used for PKA formation. It is possible to integrate this differential cross section considering the relation between atom recoil energy, $T^k$, and the scattering angle:

$$ T^k(E, \theta) = T_{\text{max}}^k(E) \sin^2(\theta/2), \quad (4.9) $$

where

$$ T_{\text{max}}^k(E) = \frac{2E(E + 2mc^2)}{M_kc^2} \quad (4.10) $$

is the maximum kinetic energy of the corresponding recoil atom, i.e., $T^k$ for $\theta = \pi$. Integrating the McKinley-Feshbach expression in the range from $T_d^k$ to $T_{\text{max}}^k$ the PKA cross section is obtained:

$$ \sigma_{\text{PKA}}^k(E) = \sigma_0(E) \cdot \left\{2\tau - 1 - \beta^2 \ln(2\tau) \pm \pi\alpha\beta \left[2\sqrt{2\tau} - \ln(2\tau) - 2\right]\right\}, \quad (4.11) $$

where $\sigma_0(E) = \pi r_0^2 Z_k^2 / \beta^4 \gamma^2$ with $Z_k$ being the atomic number of the $k$-atom, $r_0 = e^2 / mc^2$ is the electron classic radius, $\gamma^2 = 1/(1 - \beta^2)$ and $\tau = T_{\text{max}}^k / 2T_d^k$. This cross section includes the positron-atom scattering through the term involving $\pi\alpha\beta$, which takes a positive (negative) sign for electrons (positrons).

On the other hand, introducing the damage function $\nu(T)$ allows to include the atom displacement cascade phenomenon for higher atom recoil energies:

$$ \frac{d\sigma_{\text{d}}^k(E,T)}{dT} = \frac{d\sigma_{\text{McF}}^k(E,T)}{dT} \cdot \nu(T). \quad (4.12) $$

The Kinchin-Pease model (2.14) is used for the damage function in order to obtain an analytical cross section integrating this expression. Thus:
The Monte Carlo assisted Classical Method (MCCM) \[ \sigma_k^d(E) = \begin{cases} \frac{1}{2} \int_{T^k_d}^{2T^k_d} d\sigma_{\text{McF}}(E,T) \frac{dT}{dT}, & T^k_d \leq T \leq 2T^k_d; \\ \frac{1}{2T^k_d} \int_{T^k_{\text{max}}}^{2T^k_d} d\sigma_{\text{McF}}(E,T) \cdot \frac{T}{2T^k_d} dT, & T \geq 2T^k_d; \end{cases} \] (4.13)

The upper case yields \( \sigma_{\text{PKA}}^k(E) \) with \( T_{\text{max}}^k = 2T^k_d (\tau = 1) \). The second case gives the total displacement cross section including cascade processes (\( T^k \geq 2T^k_d \)):

\[ \sigma^k_d(E) = \sigma_0(E) \cdot \left\{ \tau (1 - \beta^2) + \tau \ln(\tau) + C_1 \beta^2 \pm \pi \alpha \beta \left( \tau - C_2 \sqrt{\tau} + C_1 \right) \right\}, \] (4.14)

where \( C_1 = (1 - \ln 2) \approx 0.307 \) and \( C_2 = 2(2 - \sqrt{2}) \approx 1.172 \) are calculation constants.

This expression applies then for \( E \geq E^k_c(2T^k_d) \). This is the threshold electron (positron) kinetic energy when displacement cascades start occurring. Evaluation and discussion of the displacement cross section is presented for particular cases in the following chapters.

### 4.3. Description of the simulation process

For the simulations performed within this thesis, the MCNPX version 2.6b [141] was used. This code was considered since it gives directly the fluence distribution for electrons and positrons corresponding to a given energy interval, for the flux averaged over a cell. Also, the MCNPX gives the energy deposition profiles, used to compare with the calculated dpa distributions. The simulation involves all the physical processes taking place in matter when either gamma rays or electrons pass through it (Section 3.2).

The sample geometry is defined in each case under study. This sample could then be subdivided in voxels with smaller dimensions for studying the volume and in-depth dpa distribution (figure 4.1). From the Monte Carlo simulation process, the energy fluence distributions are obtained in each defined volume. Then, the MCCM algorithm is applied to calculate the number of atom displacements in each one of them. By this way it is possible to obtain the corresponding dpa distribution profiles. The irradiation process is simulated with a large number of incident particles impacting on one of the sample...
surfaces. In all cases, the results are normalized to the total number of histories (incident photons or electrons and their secondary particles). Thus, the result is obtained as dpa per incident photon or particle source \( \frac{N_{\text{dpa}}}{\Phi_0} \). Later, knowing the source fluence or dose used in specific study, it is possible to evaluate the total number of dpa in the studied sample.

### 4.4. Working procedure for the MCCM calculations

The MCCM working procedure is summarized in figure 4.2. It uses the established Oen-Holmes-Cahn theoretical methodology for the calculation of the number of AD per electron or positron. For that the MCCM considered the McKinley-Feshbach approximation for the calculation of the displacement cross sections. On the other hand, the proposed methodology can be followed in the top of the diagram, concerning the Monte Carlo simulation. The proposal includes the preparation of all the data for the simulation through the MCNPX code, the processing of the simulation results obtaining the electron and positron fluence energy distributions and the calculation of the AD values. The comparison of the AD distributions with the energy deposition profiles (from the simulation results) is also included, with the possibility to calculate the displacements to energy deposition ratio for different energies of the incident radiation.

**Figure 4.1.:** The material volume could be subdivided in voxels for the Monte Carlo simulation process in order to calculate the dpa distributions through MCCM algorithm.
In this section some definitions and considerations in order to get more information from the fluence distributions calculated by Monte Carlo simulation and their relation with dpa and energy deposition profiles will be introduced.

First, expression (4.2) can be rewritten introducing the atom displacements rate for specific atom, $Q_k$:

$$N_{AD}^k = \int_{E_0}^{E_E} Q_k(E) \cdot \Phi_e(E) \, dE,$$  \hspace{1cm} (4.15)

with

$$Q_k(E) = N_a^k \cdot \sigma_d^{*k}(E).$$  \hspace{1cm} (4.16)

For easier analysis the following magnitudes are also introduced:

$$\Phi_k = \int_{E_0}^{E_E} \Phi_e(E) \, dE,$$  \hspace{1cm} (4.17)
The Monte Carlo assisted Classical Method (MCCM)

\[ f_k(E) = \frac{\Phi_k(E)}{\Phi_k} \], so that:
\[ \int_{E_k}^{E_0} f_k(E) \, dE = 1, \quad (4.18) \]

where \( \Phi_k \) represents the total number of electrons per cm\(^2\) in the corresponding volume or voxel, with energies in the range \([E_k, E_0]\), and \( f_k(E) \) is the probability distribution function that an electron inside the corresponding volume has energy \( E \pm dE \).

With these previous concepts:

\[ N_{AD}^k = \Phi_k \int_{E_k}^{E_0} Q_k(E) \cdot f_k(E) \, dE = \Phi_k \cdot \langle Q_k \rangle, \quad (4.19) \]

being

\[ \langle Q_k \rangle = \int_{E_k}^{E_0} Q_k(E) \cdot f_k(E) \, dE \quad (4.20) \]

the mean value of the displacements rate for the distribution function \( f_k \). From the practical point of view, this average displacements rate could be calculated if \( N_{AD}^k \) results are already known. Thus, from (4.17) and (4.19):

\[ \langle Q_k \rangle = \frac{N_{AD}^k}{\Phi_k} \cdot \langle Q_k \rangle, \quad (4.21) \]

The behavior of \( \langle Q_k \rangle \) will be defined by the distribution function of electron energies. Then, it is expected that:

\[ \langle Q_k \rangle \approx Q_k \left( \langle E_k \rangle \right) \quad \text{for} \quad \frac{\delta E_k}{\langle E_k \rangle} \ll 1, \quad (4.22) \]
where \( \langle E_k \rangle \) is the electrons mean energy for the distribution function \( f_k \) and \( \delta E_k \) is the corresponding standard deviation:

\[
\langle E_k \rangle = \int_{E_k^L}^{E_k^H} E \cdot f_k(E) \, dE, \quad (4.23)
\]

\[
\delta E_k = \left[ \int_{E_k^L}^{E_k^H} (E - \langle E_k \rangle)^2 \cdot f_k(E) \, dE \right]^{1/2}. \quad (4.24)
\]

On the other hand, the energy deposition \( (E_{\text{dep}}) \) profiles are also calculated for each studied case. These profiles are then compared with the corresponding atom displacements distributions in order to establish an energy deposition to atom displacements relation. This way the displacements to energy deposition ratio, \( \eta(E_0) \), can be introduced for a given incident radiation energy.

All these previous analytical tools are useful for analyzing and discussing the in-depth atom displacements profiles.

### 4.6. Implemented calculation tools

To ease the application of the MCCM some tools were developed. First a dynamic link library (DLL) with many functions with external access was implemented. Later, a graphical user interface (GUI) tool, that allows easy handling of the various features included in the library, was also developed.

#### 4.6.1. MCCM functions library

The MCCM DLL was implemented using the C++ programming language. File management was implemented using the eXtensible Markup Language (XML), which is a meta-markup language that provides a format for describing structured data. It plays a very important roll today because it allows compatibility between systems to share information in a secure, reliable and easy way. The DLL contains 45 user interface functions at this moment (further details in [142]).
The MCCM DLL uses handles, each one corresponding to a fluence distribution for one specific calculation. Each MCCM handle consists in three main groups of data:

- **FluenceData** - values of the electrons and/or positrons energy fluence distributions (cm\(^{-2}\)), including the quantity of distributions (number of cells used in the simulation) and the length of each of them (number of energy bins),

- **Material** - all the characteristics of the studied material (name, formula, density, dimensions, values of displacements energy for each atom, etc.),

- **Ndpa** - values of the atom displacements distributions, calculated for electrons and positrons in each cell of the material.

The built Windows based GUI application was development in MS Visual Basic environment. With this tool it is possible to set all the needed data and characteristics, to process MCCM XML documents or MCNPX output files, and to define a material giving all their properties. Furthermore, users can also evaluate the displacement cross sections for all atoms in the defined material in the selected energy range.

### 4.6.2. MCCM graphical user interface

The built Microsoft Windows system based GUI application (figure 4.3) was development in Microsoft Visual Basic environment. With this tool it is possible to set all the data and characteristics. Besides, an existing full XML document or an output file containing all simulation results from MCNPX can be processed. It is also possible to import the flux data and/or the material from a predefined XML file. In a similar way the Fluence Data, Material and/or Ndpa can be exported to an XML file for future uses. With this GUI it is possible to define any material giving all their properties and characteristics.

Then it is possible to perform the dpa calculations when all the data are completely and correctly set. Furthermore, a detailed report of the results can be obtained containing all the properties and characteristics of the calculation process. The user can also evaluate the displacement cross sections for all atoms in the defined material in the selected energy range and/or export the calculated displacement cross sections data to a file. Further information about this tool can be found in [143,144].
Figure 4.3.: Main interface of the MCCM GUI tool.
Chapter 5.

Comparing MCCM with the previous calculations

“A person who never made a mistake never tried anything new.”
— Albert Einstein (1879–1955)

Oen and Holmes [3] calculate the cross sections for the displacement of lattice atoms by gamma rays with energies up to 5 MeV. They analyzed different gamma interaction processes with matter leading to secondary electron generation. The principal contribution is found to come from the Compton effect, when the atoms are displaced by the gamma rays produced electrons. Several authors had estimated the dpa cross sections under different approximations and models, including most of the gamma-material interaction processes [4,13,54,101,104,145,146]. The common conclusion is that the main contribution to dpa cross section comes from the Compton effect for lighter and medium elements and for energies up to about 10 MeV.

On the other hand, no exact analytical formula covering the whole energy range is available for the differential cross section for producing an electron or a positron in the cases of photoelectric effect and pair production processes. The previous works used numerical approximation formulas which are applicable for limited energy ranges. For all this, is common to use the Klein-Nishina analytical expression [147] for the Compton effect to perform dpa calculations.
In this chapter, a comparison of the MCCM procedure with previous classical calculations is analyzed. The main difference is related to the secondary particle spectra considered for calculations, which depends on the incident radiation nature and on its interaction processes with the material.

5.1. Secondary particle fluence distribution

First, some analysis of the calculated energy fluence distributions from the Monte Carlo simulation is presented. For the calculations the material and experimental conditions used by Belevtsev and coworkers in [13] are employed. They used the theoretical Compton electrons distribution to estimate the dpa cross section in YBCO by gamma irradiation with a $^{60}$Co source. Then, the analytical energy distribution of Compton electrons is compared to the energy distributions used by MCCM. In this sense, the effective fluence of ejected Compton electrons is evaluated, following [13, 71], according to:

$$\Phi_C(E) = \frac{\Phi_\gamma N_a}{(-dE/dx)} \int_{E}^{E_{\text{max}}} \sigma_C(E') dE' ,$$  \hspace{1cm} (5.1)

where $\Phi_\gamma$ is the $\gamma$-ray incident fluence, $(-dE/dx)$ is the energy loss per cm of electron path, $E_{\text{max}} = 2E_\gamma^2/(mc^2 + 2E_\gamma)$ is the Compton electron maximum energy, with $E_\gamma$ being the photon energy in a monoenergetic $\gamma$-ray fluence, and $\sigma_C(E)$ is the cross section per atom for a Compton electron production at energy $E$ [147], expressed as:

$$\sigma_c(\varepsilon) = \sigma_0 \left\{ \frac{1}{1-\varepsilon} + 1 - \varepsilon + \frac{\varepsilon}{g^2(1-\varepsilon)} \left[ \frac{\varepsilon}{1-\varepsilon} - 2g \right] \right\} ,$$ \hspace{1cm} (5.2)

with $\varepsilon = E/E_\gamma$, $g = E_\gamma/mc^2$ and $\sigma_0 = \pi r_0^2 Z mc^2/E_\gamma^2$.

In the case of MCCM, the whole electron fluence energy distributions inside the sample are obtained from the Monte Carlo simulation of radiation transport through matter. This distribution is calculated for a gamma incident energy of 1.25 MeV ($^{60}$Co averaged energy). Fluence distributions for incident gamma energies below (662 keV from a $^{137}$Cs source) and above (3 MeV) are also computed. Figure 5.1 shows these results, where the corresponding normalized effective electron fluence values are calculated from the MCCM resulting original fluence values.
Comparing MCCM with the previous calculations

Figure 5.1.: Normalized effective electron energy fluence distributions for three incident gamma energies. The distributions obtained by MC simulation inside the sample are shown (in black). The theoretical distribution of Compton electrons is also included (continuous red curves). Yellow and hatched regions correspond to the dpa integration interval ($E_k^c \rightarrow E_{\text{max}}$) for simulated and Compton distributions respectively.

An interesting fact is related to the shape of these distributions. First, the ejected photoelectrons can obtain the highest kinetic energy values (close to $E_\gamma$) with an appreciable relative intensity for lower incident energies, which may give an important contribution to dpa values. In addition, the continuous electron contribution arising from Compton scattering, as well as from the relaxation processes, becomes a broader single-mode distribution when increasing $E_\gamma$ values, with a width near to the maximum Compton electrons kinetic energy.

The continuous red curves in figure 5.1 represent the calculated distribution of effective Compton electrons fluence through expression (5.1). These values are also normalized to incident gamma fluence for better comparison. The region in yellow indicates the fluence of particles that contribute to the formation of oxygen displacements in the YBCO material ($E_k^c \approx 130$ keV). This is the region that is integrated in equation (4.5) to calculate dpa values, i.e., this area is in fact the $P_k$ values in each case (Eq. (4.17)). The hatched region means the same, but for the analytical Compton distribution. Analyzing this, some interesting conclusion can be drawn. It is easy to note the difference between simulated and analytical distributions, corresponding to the primary Compton part of the fluence spectrum.
Comparing MCCM with the previous calculations

For the gamma energy at 662 keV an underestimation of the theoretical effective fluence compared to the simulated one is observed (about 69%). In this case the contribution of the calculated Compton distribution to dpa formation is about 76% of the corresponding simulated one. For lower gamma energy (i.e. 122 keV, not included in figure 5.1) the contribution from Compton electrons to the generated effective fluence inside the material is quite small (~4%). For photons with 1.25 MeV energy a better agreement between the Compton part of the spectrum with the simulated one is observed. In this case the analytical distribution overestimates the simulated one with about 6%. The contribution to dpa formation from Compton is about 9% higher relative to the simulated one for this energy.

For higher incident energy more photons and secondary particles will escape from the sample, since the mean free path for photons and electron’s ranges are higher. For example, the mean free path for photons with 1.25 MeV is about 4 cm (electron range about 1.5 mm) and about 24% of the primary does not interact with the target sample, which is 2.2 cm width in this calculations, like in [13]. In this case, not all photons from the source will interact inside the sample and neither do all the produced secondary electrons. The Compton energy range of the fluence spectrum will be wider for higher gamma energies, since $E_{\text{max}} \approx E_\gamma$. However, pair production interaction processes will appear and increase in importance with increasing gamma energy. For 3 MeV incident gamma energy the contribution from the primary Compton electron part is also higher than the simulated one by about 33%, contributing with more than 43% to the dpa calculation.

5.2. Dpa induced by gamma irradiation

Taking the previous works reported on the estimation of the dpa cross sections for gamma induced displacements in some materials as a reference, the MCCM procedure is applied and both results are compared. It is good to clarify that all the simulations for this comparisons were performed for large material dimensions (3 cm $\times$ 3 cm $\times$ 3 cm). This way it is ensured that the maximum number of photons and electrons interact inside the material. It minimizes the underestimation from our calculations due to small material sample sizes. The key for all those previous “classical” estimations is to assume that the electrons are stopped inside the solid sample. In addition, positrons are considered as electrons in these calculations, as was done in all previous estimations, with exception of
Comparing MCCM with the previous calculations

Cahn [4] and Fukuya and Kimura [54]. Despite all this, in general, one can expect an overestimation from these “classical” approaches, since they are based on analytical and numerical distributions for the gamma-material interaction processes on infinite media, considering that all primary photons interact with the target material.

We start with the work from Oen and Holmes [3], a classic in this topic, in which they proposed the methodology explained in Section 2.5 for the calculation of dpa cross sections. They presented the calculation of the dpa cross section by gamma rays through the Compton process as function of the incident gamma energy for elements with $Z=4, 29, 92$ for different displacement energies. The corresponding dpa cross sections for Cu through MCCM for two displacement energies are presented in figure 5.2 together with their results for better comparison. A good agreement is seen between our calculations and those from Oen and Holmes. As it was expected there is an overestimation from their results for lower energies. Their results are higher in about 10-40\% than ours for incident gamma energies up to 2.5 MeV in the case of $T_d=15 \text{ eV}$ and 10-90\% in the case of $T_d=25 \text{ eV}$. For energies higher than 3 MeV their underestimation is consequence of considering only the Compton processes, and it is known that for higher energies the pair production process is dominant. Also, they do not included in their calculations the AD cascade phenomena that becomes important at higher energies.

Cahn also applied the same procedure to estimate the dpa cross sections in Si and Ge under gamma irradiation up to 7 MeV [4]. He included the three main gamma-material interaction processes and the cascade phenomenon in his calculations. Our results through MCCM and Cahn’s are presented in figure 5.3 for Si using two values of the displacement energy. An overestimation in his calculations is noted, being about 1.1-1.4 times our results for $T_d=15 \text{ eV}$. For $T_d=30 \text{ eV}$ that difference is a bit higher, about 1.2-1.9. It is then found that this overestimation decreases for higher incident gamma energies and for lower displacement energies.

Something different happens with the results of Kwon and Motta [104]. Their results for Si and the corresponding ones from MCCM are presented in figure 5.4. Their calculations overestimate ours with factors 1.1-2.5 ($T_d=24 \text{ eV}$) and 1.2-3.6 ($T_d=40 \text{ eV}$) times up to 5 MeV incident gamma energy. For higher gamma energies Kwon-Motta’s cross section shows a more gentle energy dependence, with a difference of only 2\% ($T_d=24 \text{ eV}$) and 9\% ($T_d=40 \text{ eV}$) relative to ours for 10 MeV incident energy. Such gentle energy dependence is probably because the displacements by positrons was neglected in their calculations.
Comparing MCCM with the previous calculations

Figure 5.2.: Dpa cross sections calculated by Oen and Holmes [3] and MCCM in Cu for two values of the displacement energy.

Figure 5.3.: Dpa cross sections in Si estimated by Cahn [4] and calculated by MCCM for two values of the displacement energy.

Figure 5.4.: Dpa cross sections in Si according to Kwon and Motta [104] and MCCM for two values of the displacement energy.

Figure 5.5.: Dpa cross sections in Fe by Fukuya-Kimura [54], Kwon-Motta [104], Baumann [101], Alexander [146] and MCCM.
Some other estimations of dpa cross sections have been done in Fe by several authors. Figure 5.5 shows those results for different displacement energies and approximations, together with our results through MCCM for 25 eV and 40 eV displacement energies for comparison. All these authors considered photo-electric effect, Compton and pair production processes in the calculation of the dpa cross sections. The Kwon and Motta calculations were discussed above and the same comments apply for Fe. Higher difference for lower energies is obtained (1.5-7.6 times) since they used $T_d=24$ eV and our calculations in this case are based on $T_d=25$ eV. The estimations by Fukuya and Kimura [54], using the Kinchin-Pease model for the damage function, are 1.2-1.5 times higher than ours. They considered both electrons and positrons, concluding that it results in a reduction by a factor of 1.1 compared to an approximation treating a positron as an electron, as considered in our calculations.

For the case of $T_d=40$ eV, the calculations by Baumann [101] gave higher dpa cross sections by a factor of 1.4-2.6 than the present calculation. He used Oen’s tabulated electron-induced cross sections [102]. The difference with the results by Alexander [146] is smaller, just about 1.2-1.3 higher than MCCM calculations. He used the same differential PKA cross section (McKinley-Feshbach approximation), but using the NRT model [64] for the damage function. Fukuya and Kimura concluded that the NRT model gave results that are 1.3 times smaller than the Kinchin-Pease model for Fe [54].

Last, the results from Belevtsev et al. [13] are analyzed. They used the methodology discussed in the previous section to estimate the dpa cross section induced in YBCO by gamma irradiation with $^{60}$Co source. Their results are about 2.8 higher than ours. As discussed in the previous section this overestimation is partly because their sample width of 2.2 cm is used here.

### 5.3. Dpa induced by electron irradiation

Oen and Holmes [3] and Cahn [4] also calculated the number of displacements per incident electron in some metals for different displacement energies through (2.13). In order to compare with their results the expression (4.2) is used.

Simulations for different incident electrons energies are then performed, considering large material dimensions, to ensure that most of the incident electrons interact inside the
Comparing MCCM with the previous calculations

Material. This way the results will be consequent with the “thick target” approximation assumed in (2.13) in order to have a fair comparison.

Their results and those through MCCM for Cu and Si and displacement energies used in previous mentioned works are presented in figures 5.6 and 5.7. A good agreement between our calculations and those from Oen and Holmes is found. MCCM calculations are about 2-6% higher than their estimations for electron energies about 1 MeV. For higher electron energies, the difference increases up to 50% in the case of $T_d = 15$ eV and $\sim 40\%$ for $T_d = 25$ eV for electron energies about 5 MeV. The underestimation of their results is related to the fact that their calculations considered displacements induced by an electron along its path in the material, but they do not take into account the secondary particles produced in the electron-material interaction processes. On the contrary, all those processes are included in the Monte Carlo simulation performed in the framework of MCCM. Also, for higher energies their underestimation is consequence of ignoring the AD cascade phenomenon.

Cahn’s results show good agreement with MCCM for all electron and displacement energies, with an underestimation in his calculations that decreases for higher electron energies, being about 5-36% relative to our results in the studied energy range. This underestimation is up to 5% lower for $T_d = 30$ eV than for $T_d = 15$ eV. For higher electron

![Figure 5.6.](image1.png) ![Figure 5.7.](image2.png)

**Figure 5.6.** Number of displacements per electron calculated by Oen and Holmes [3] and MCCM in Cu for two values of $T_d$.

**Figure 5.7.** Number of displacements per electron in Si estimated by Cahn [4] and calculated by MCCM for two values of $T_d$. 
Comparing MCCM with the previous calculations

energies, near 7 MeV, Cahn’s underestimation is even a factor 1.1 times below our results. This could be a consequence of the approximation used by Cahn for the stopping power evaluation. He used empirical range-energy formulas [148], which present different energy-dependence for higher energies than the one used in MCNPX and MCCM.

The MCCM results are now compared with some other previous estimations of dpa induced by electron irradiation in thin samples. Starting with the work by Basu et al. on electron-beam-irradiation effects in bulk YBa$_2$Cu$_3$O$_{7-x}$ [149]. They studied irradiation effects in a transmission electron microscope using 100-300 keV electrons. They found that YBCO is insensitive to 100 keV electrons, indicating that the displacement energy should be higher than 15 eV. They estimated displacements per atom values for oxygen atoms only as the product of the Oen’s cross section [102] (with $T_d=18$ eV) and the fluence used for irradiation. This evaluation results in an overestimation since Oen’s calculations assume that the electrons come to rest within the solid sample. Basu et al. analyzed thin foils of YBCO in form of 30 µm thick slabs. The energies they used lead to electron ranges of about 45 to 250 µm. Their experiments are simulated and the dpa values through MCCM are calculated. Results are presented in Table 5.1. Their results are 1.2-1.4 times higher than our calculations for energies 200-300 keV, being 3.2 times higher for lower energies of 150 keV. Then, their results are overestimated between 20% and 69% for the studied electron energies.

Table 5.1.: Electron-irradiation induced dpa values estimated in previous works and those calculated through MCCM. The relative difference between them is also showed.

<table>
<thead>
<tr>
<th>Ref.</th>
<th>$E_0$ (MeV)</th>
<th>dpa in Ref.</th>
<th>dpa in MCCM</th>
<th>Rel. diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basu et al. [149]</td>
<td>0.15</td>
<td>1.51</td>
<td>0.47</td>
<td>69%</td>
</tr>
<tr>
<td></td>
<td>0.20</td>
<td>2.10</td>
<td>1.50</td>
<td>29%</td>
</tr>
<tr>
<td></td>
<td>0.25</td>
<td>2.99</td>
<td>2.40</td>
<td>20%</td>
</tr>
<tr>
<td></td>
<td>0.30</td>
<td>3.38</td>
<td>2.68</td>
<td>21%</td>
</tr>
<tr>
<td></td>
<td>3.76</td>
<td>2.99</td>
<td>20%</td>
<td></td>
</tr>
<tr>
<td>Giapintzakis et al. [58]</td>
<td>0.35</td>
<td>2.05-10^{-4}</td>
<td>1.30-10^{-4}</td>
<td>37%</td>
</tr>
<tr>
<td></td>
<td>8.19-10^{-4}</td>
<td>5.20-10^{-4}</td>
<td>37%</td>
<td></td>
</tr>
<tr>
<td>Yacoby et al. [150]</td>
<td>2.50</td>
<td>5.00-10^{-4}</td>
<td>2.36-10^{-4}</td>
<td>53%</td>
</tr>
<tr>
<td></td>
<td>1.00-10^{-3}</td>
<td>5.07-10^{-4}</td>
<td>49%</td>
<td></td>
</tr>
</tbody>
</table>
Giapintzakis et al. [58] used 350 keV electrons to study point defects in YBCO single crystals. They calculated dpa values in a way similar to that previously explained, using $T_d=20$ eV and different electron fluences, obtaining $2.05 \times 10^{-4}$ and $8.19 \times 10^{-4}$ dpa. Their sample is even thinner, with 9 $\mu$m width, and electrons with 350 keV energy have about 318 $\mu$m of range in YBCO. Their experiment is also simulated and the dpa values for both fluences in the sample are calculated, resulting in $1.30 \times 10^{-4}$ and $5.20 \times 10^{-4}$ dpa respectively, values about 1.6 times lower than their estimations. The overestimation in their results is then $\sim 37\%$.

Another study in which the authors tried to evaluate dpa induced by higher energy electrons (2.5 MeV) is the one carried out by Yacoby and coworkers [150]. They investigated the effect of two doses of 2.5 MeV electron irradiation on the irreversibility line of a ceramic YBCO sample. They also estimated dpa values using Oen’s cross sections for $T_d=20$ eV for all atoms in the material. Their sample is 100 $\mu$m width, but electrons with 2.5 MeV have penetration $>3$ mm. Their experiment is simulated and the corresponding dpa values are calculated. The results through MCCM are 2.0-2.1 times lower than their estimations (Table 5.1).

### 5.4. Chapter conclusions

The MCCM results were compared with previous theoretical calculations in this chapter. The main difference was found to be related to the secondary particle spectra considered for calculations, which depends on the incident radiation nature and on its interaction processes with the material. The difference between the calculated analytical distributions and the simulated ones is remarkable. The simulation process gives a more realistic approach by taking into account the material dimensions and all interaction and transport processes of photons and electrons/positrons in matter.

A good agreement between our calculations and those from Oen-Holmes and Cahn established methodologies was observed for the analyzed electron and displacement energies. An overestimation in about 10-90% for the gamma irradiation induced dpa cross section from the previous evaluations was observed on regard to the MCCM results. On the contrary, the dpa cross section values produced by irradiation with electrons are underestimated in about 5-50% by the “classical” approximations when compared to the MCCM calculations. When thin samples are irradiated with electrons, the previous
established methodologies lead again to an overestimation in about 20-70% related to the more precise results obtained through the MCCM.

Therefore, the complex behavior of the gamma and electron interaction processes with matter cannot be neglected at all for dpa calculations. The MCCM methodology supports the introduction of a more realistic treatment for gamma and secondary electron/positron transport as demonstrated here with Monte Carlo based simulations. MCCM also allows to evaluate and study the dpa volume distributions inside the target material.
Part III.

Results calculating the displacements per atom distributions in some technologically interesting materials
Chapter 6.

Dpa distributions in YBCO superconducting material

“The scientist is not a person who gives the right answers,
he’s one who asks the right questions.”
— Claude Lévi-Strauss (1908–2009)

This chapter is closely related with the results presented in the following publications:

- I. Piñera, C. M. Cruz, P. Van Espen, Y. Abreu, A. Leyva

- C. M. Cruz, I. Piñera, A. Leyva, Y. Abreu

- I. Piñera, C. M. Cruz, Y. Abreu, A. Leyva, A. E. Cabal, P. Van Espen

- I. Piñera, C. M. Cruz, Y. Abreu, A. Leyva

- I. Piñera, C. M. Cruz, A. Leyva, Y. Abreu

- I. Piñera, C. M. Cruz, Y. Abreu, A. Leyva
6.1. Introduction

Among the most interesting materials, due to their applications in many science and technology fields, are the high-temperature superconductors (HTS’s) [151–158]. An enormous amount of work has been done on the study of defects and their effect on the HTS’s properties. It is believed that these studies may provide the key to understanding their properties and offer some insight into the mechanism of high-Tc superconductivity. Recent investigations have found copper oxide superconductors to be very sensitive to damage caused by irradiation with highly energetic particles [159–162] and with gamma rays [163–170].

One of the more representative cases within this group is the high-temperature ceramic superconductor YBa$_2$Cu$_3$O$_7$ (known as YBCO). Since the discovery of the YBCO much effort has been spent on studying it. This effort is motivated by its potential use to attain new fundamental knowledge on this unique material and the clarification of its superconductive mechanism. Also, it is easy and cheap to obtain and it promises interesting technological applications [171–187].

The Radiation Damage group at CEADEN has also been investigating YBCO ceramic superconductors under irradiation since several years. The energy deposition and the transition temperature depth profiling of gamma-irradiated YBCO ceramic were studied in [188,189]. The broadening of the grain boundary induced by gamma radiation was also investigated [190]. Another study analyzed the $^{57}$Fe Mössbauer spectra interpretation regarding doped YBCO samples [191]. Some other studies deal with the radiation damage evaluation on this material by means of Monte Carlo simulation [35–37,41].

This chapter presents the results related to Monte Carlo based simulations supporting the calculation of the atom displacement processes induced by gamma and electron irradiation on YBa$_2$Cu$_3$O$_7$ HTS material.

6.2. Selection of the threshold displacement energy

First, it is necessary to discuss previous reports concerning the threshold displacement energies in YBCO. As it is well-known, the main crystalline sites on regard to transport properties and superconductivity in the YBCO material are the Cu-O$_2$ (planar) and Cu-O (chain) sites (figure 6.1), which have been studied by several authors.
Observing visible defect formation in several in-situ Transmission Electron Microscopy (TEM) studies it might be suggested that the incident electron energy needed to displace a chain oxygen is $\sim 130$ keV [149, 192]. The threshold energy absorbed to displace an oxygen atom is therefore 20 eV (from (2.1)). Matsunami et al. [193] also assumed that $T_d = 20$ eV for oxygen in Bi-based HTS oxides, as Barbour et al. [194] did in Tl-2223 HTS oxides. These HTS oxides have nearly the same structure and include the same or similar elements (O, Cu and heavy atoms). Accordingly, $T_d$ is assumed to be nearly the same for these oxides.

Giapintzakis et al. [195] have reported that the pinning capability of YBCO crystals was enhanced only if the energy of the incident electron beam was greater than 500 keV. They suggested that this was the threshold incident electron energy for producing displacements of copper atoms from the CuO$_2$ planes, so $T_d(Cu) = 25$ eV.

On the other hand, critical temperature degradation at the very initial stage was observed at smaller $T_d$ ($\sim 10$ eV) [19]. Cui et al. [196] performed molecular-dynamics simulations based on a pair potential model and also found that the planar oxygen...
displacement threshold may be as low as about 10 eV. In later investigations on the anisotropy of $T_d$, Cui et al. [197] showed that the displacements of the oxygen atoms will lie preferentially in the basal (001) plane, obtaining $T_d$ values of 4.2 eV and 18.8 eV for the basal plane (001) and (100) respectively. By analyzing the changes in properties at different energies of incident electrons, Tolpygo and coworkers [198] have found the threshold energy for displacement of oxygen on Cu-O$_2$ planes and evaluated the displacement energy for plane oxygen as 8.4 eV. Giapintzakis et al. [58] felt that these low threshold values may not be so accurate, since several TEM experiments at 100 keV ($T_d$(O)=15 eV) has shown no evidence for displacement damage in this material [149,192]. The observation of different effects could be a reason for the above discrepancy.

Tolpygo et al. [198] also estimated the upper limit on the displacement energy for chain oxygen as 2.8 eV. Bourdillon and Tan [199], estimated from thermodynamic data, estimated 3.45 eV as an upper limit for the displacement energy of chain oxygen.

To summarize, in the case of the planar sites displacement energy values of 20 eV for oxygen and 25 eV for copper atoms have been obtained experimentally [58,149], which are the most used values for these atoms. Then, these are the values selected for the studies presented here. In the case of chain oxygen the Bourdillon and Tan’s value of 3.45 eV is chosen. Not any experimental report about the yttrium and barium atoms for this material was found. Thus, taken into account the previous considerations, the standard value of 25 eV is selected for these atoms; however several studies indicate that it should be higher.

6.3. Dpa in planar and chain sites under low gamma irradiation

In this kind of study, it is necessary to take into account the specific atom that will be displaced and the position that it occupies in the crystalline lattice. It is well-known that the oxygen atoms are more liable to be taken out of their crystalline sites because they are the lightest. Two crystalline positions for the oxygen atoms in this material are discussed, the Cu-O chains and Cu-O$_2$ planar sites (figure 6.1). Tolpygo et al. [200] concluded that the increase of both the T-linear resistivity slope and the Hall coefficient of YBCO is also due to the formation of defects in chains which occurs simultaneously with the formation of in-plane defects; but the critical temperature ($T_c$) suppression is primarily
due to in-plane defects. Giapintzakis et al. [58] also found that oxygen displacements from the Cu-O$_2$ planes rather than the chains are the dominant contribution to the irradiation-induced suppression of $T_c$.

In this section the oxygen dpa distributions in both chain and plane crystalline sites at low gamma irradiation energies are analyzed. Based on previous studies [188,189], $^{57}$Co, $^{137}$Cs and $^{60}$Co sources ($E_\gamma = 122$ keV, 662 keV and 1250 keV respectively) are used in this case.

Figure 6.2(a) shows the dependences of the displacement cross section $\sigma_d$ on $T_d$ for the three incident gamma radiation energies of interest. These values are the feasible maximum kinetic energies of the corresponding secondary electrons. For electron kinetic energies of 122 keV, the maximum kinetic energy of recoil atoms is $\approx$ 18.6 eV (where $\sigma_d$ vanishes in this figure). This means that in this kinetic energy range, the secondary electrons will not induce displacements on O(2-3) crystalline sites defining the Cu-O$_2$ planes, with an assumed $T_d = 20$ eV. On the contrary, displacements in the O(4) Cu-O chain sites will be allowed for electron kinetic energies lying well below 122 keV with an assigned $T_d = 3.45$ eV. Chain O(1) it is not included because only the defects in the basal plane “ab” are important for superconducting transport properties.

Figure 6.2.: Displacement cross sections (a) as function of displacement energy for different incident energies and (b) as function of electron kinetic energy for both chain and planar sites (dashed lines correspond to PKA cross section).
The dependencies of $\sigma_{PKA}$ and $\sigma_d$ on the electron kinetic energies are shown in figure 6.2(b), for the two used values of $T_d$, related with oxygen crystalline sites. As it was expected, both cross sections vanish below a certain value of the incident electron energy. In case of $T_d = 20$ eV, this value is about 130 keV and for $T_d = 3.45$ eV is about 25 keV. These values are precisely the cutoff kinetic energies of electrons for displacing oxygen atoms with those $T_d$ values (Eq. (4.6)).

The setup of the sample geometry and irradiation conditions for simulations was selected similar to those used in previous studies [188, 189]. The ceramic YBCO parallelepiped target was shaped with dimensions 2.8 mm $\times$ 16.0 mm $\times$ 1.5 mm (subdivided in voxels with 0.4 mm $\times$ 0.4 mm $\times$ 0.1 mm), on which $10^8$ photons impacted at different selected incident energies (122 keV, 662 keV and 1250 keV). The relative errors in all simulation results were always below 3%.

Expression (4.5) is applied to both types of oxygen atoms in YBCO: (A) oxygen atoms O(2-3) sited in the Cu-O$_2$ planes ($k = O_p$) with $T_d = 20$ eV and $n_{O_p} = 4/13$; and (B) oxygen atoms O(4) sited in the Cu-O chains ($k = O_c$) with $T_d = 3.45$ eV and $n_{O_c} = 1/13$. These results are shown in figure 6.3 for both (A) and (B) cases and for the three selected $E_\gamma$ values. In all the cases dpa values are normalized to be per incident source photons.

**Figure 6.3.** Dpa in-depth distributions for oxygen atoms in the Cu-O chain and Cu-O$_2$ planar sites of YBCO superconductor.

**Figure 6.4.** Total oxygen dpa for each incident gamma energy in Cu-O chain and Cu-O$_2$ planar sites of YBCO superconductor.
It is good to mention that in all figures presented within the results the continuous lines represent a visual guide, excepting the cases when something different is specified.

From this calculation the contribution from the $O_c$ atoms to the total calculated dpa value dominates at all $z$ positions, in the selected range of $E_\gamma$ values, although $n_{O_c} < n_{O_p}$. This peculiar dpa behavior in YBa$_2$Cu$_3$O$_{7-x}$ relies on the different values of the displacement cross section (see figure 6.2(b)), calculated for $T_d = 3.45$ eV ($O_c$) and $T_d = 20$ eV ($O_p$), favoring the displacement phenomenon in the Cu-O chains. The dpa in-depth distributions are unimodal, showing a maximum inside the sample at deeper position as the gamma energy increases. One can also notice the relative homogeneity of gamma damage in the whole volume of the sample, being better for lower energies. The relative difference between minimum and maximum dpa values through the sample for chain oxygen is about 38% for 122 keV incident energy, increasing for 662 keV (50%) and 1250 keV (72%). For oxygen in planar sites this difference is about 52% (662 keV) and 74% (1250 keV).

The total dpa value in the sample can be estimated averaging all voxel values for each incident energy in the whole volume (figure 6.4). For $E_\gamma = 1250$ keV (average from $^{60}$Co source), which is usually taken as reference gamma irradiation source, the higher value about $10^{-27}$ dpa per incident photon is obtained, with a contribution from $O_c$ atoms of about 80% to the total dpa. The contribution in the case of 662 keV incident gammas is slightly higher $\sim$86%, and for 122 keV all displacements are from chain sites. It is interesting that the total dpa produced by 122 keV incident radiation is about 1.07 times higher than those induced in the case of 662 keV irradiation. This can be attributed to the low displacement energy value for the chain sites, leading to low cutoff electron energy (25 keV). As was discussed previously, a larger number of low energy electrons are produced by lower gamma energy irradiation. Then for low $T_d$ value most of those electrons contribute to dpa formation. Besides, most of the electrons are produced via the photo-electric effect, since Compton electrons have a maximum energy ($\sim$39 keV) close to the cutoff energy. Also, the photo-electric effect has an interaction cross section about five times higher than the one for Compton scattering at 122 keV for YBCO. As a consequence the total $\Phi_k$ value calculated for 122 keV incident gamma energy is about 1.12 times the one obtained for 662 keV.

Some known experimental studies of single-crystal HTS’s irradiated with electrons or ions show that an appreciable influence of disorder on resistivity and $T_c$ can be detected only at dpa greater than $\approx 10^{-3}$ [58,201,202]. A high gamma irradiation fluence $\geq 10^{24}$ photons/cm$^2$ will then be needed. However, Belevtsev et al. [13] observed a pronounced
effect of typical \( \gamma \)-rays doses (\( \sim 10^{17} \) photons/cm\(^2\)) on \( T_c \) and the width of resistive transition. They concluded that this is undoubtedly connected with the influence of \( \gamma \)-rays on poor conductive or dielectric regions of grain boundaries and, therefore, on the superconducting phase coherence between the grains. Some other studies found such results using not too much higher doses [203, 204]. Even, Leyva \textit{et al.} found an increase of the transition temperature for lower doses of \( ^{60} \text{Co} \) (up to 600 kGy) and \( ^{137} \text{Cs} \) (up to 500 mGy) gamma-rays sources for \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_x \) superconducting rods [205]. In another similar study they found such results for YBCO ceramic for even lower dose (265 mGy) of \( ^{137} \text{Cs} \) gamma-rays source [189]. Considering this dose, our results through MCCM give a total of about \( 10^{-18} \) dpa, then supporting the conclusions from Belevtsev and coworkers.

6.3.1. Correlation between dpa and energy deposition

The in-depth energy deposition profiles were also calculated through Monte Carlo simulation for all studied incident gamma energies (figure 6.5).

As can be observed from this figure, energy deposition profiles have similar in-depth shape than corresponding dpa distributions. It can be noted that energy deposition is

![Figure 6.5: In-depth energy deposition profiles for three gamma radiation energies on YBCO.](image1)

![Figure 6.6: Dpa dependence with energy deposition for three gamma ray energies. Continuous lines represent a linear fit to the data.](image2)
higher for 122 keV incident photons, since for higher energies lower number of incident photons interact inside the sample, because of the high penetration of the gamma radiation. This supports the fact that the total dpa for 122 keV is higher than for 662 keV irradiation, as it was observed in figure 6.4.

Based on the similarity between dpa and energy deposition distributions a comparison is performed through figure 6.6. The correlation among these profiles can be evaluated through the non-parametric Spearman coefficient, giving large values about 0.70-0.99, significant at the 95% level, for the studied incident energies. It seems from figure 6.6 the nearly linear dependence between dpa and energy deposition for each incident energy. Then a linear fit to these dependences is performed in order to obtain the dpa to energy deposition ratio, $\eta(E_0)$, for each incident gamma source. The results are presented in Table 6.1, confirming that the gamma radiation energy deposition process in YBCO material supports better the displacement production at higher incident energies.

These findings seem to confirm partially the results reported by Leyva et al. [189], in which the calculated energy depositions were taken as a measurement of the gamma radiation damage effects on the YBCO superconducting material.

### 6.4. Dpa profiles for higher energy gamma irradiation

Here, the results of the dpa distribution determination in YBCO induced by gamma irradiation with an initial energy up to 15 MeV are presented. For higher incident energies, displacements of the heavier atoms will also occur. Then, the contribution to the total dpa distribution from each one of the four atoms that compose the material is analyzed in this study.
In the case of the oxygen and copper atoms only the planar site is now considered. The transport of charge carriers occurs in the Cu-O\(_2\) planes and thus the interactions of these carriers will be predominantly with the defects that are located in the planar sites. On the other hand, the dpa cross section for oxygen and copper atoms in the chains are higher than in the planar sites at low particle energies. However, when increasing energy, the cross section for primary dpa in chains decreases and the corresponding one for atoms in planes increases (figure 6.2). Furthermore, there is evidence in the literature that the defects that induce changes observed in some characteristic properties of this material, like T\(_c\), are those that take place in the planar sites [58, 59, 198, 206–208].

Figure 6.7 shows how the cutoff electron kinetic energy depends on the displacement energy for each atom of YBCO. For the assumed T\(_d\) values then displacements will occur for electron energies higher than \(\sim\)130 keV in the case of oxygen atoms. Cu, Y and Ba displacements will be produced for electron energies \(\geq\)492 keV, 631 keV and 857 keV respectively (Table 6.2). It can also be deduced from here that multiple displacements will start occurring for electron kinetic energies about 238 keV, 813 keV, 1.02 MeV and 1.35 MeV for O, Cu, Y and Ba atoms correspondingly.

The dependence on electron kinetic energy of the maximum kinetic energy of recoil atoms is plotted in figure 6.8. The inset shows the low energy region. It can be noticed

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**Figure 6.7.**: Cutoff electron kinetic energy for different displacement energies for all atoms in YBCO.

**Figure 6.8.**: Maximum kinetic energy of recoil atoms in YBCO. Dashed lines in the inset indicate values of \(E=662\) keV and \(T_{\text{max}}=25\) eV.
Table 6.2: Values of $T_d$ and $n_k$ used to calculate $N_{dpa}$. The cutoff electron kinetic energies and the maximum kinetic energies of recoil atoms are also presented.

<table>
<thead>
<tr>
<th>Atom</th>
<th>k</th>
<th>$n_k$</th>
<th>$T_d^k$ (eV)</th>
<th>$E_c^k$ (keV)</th>
<th>$T_{max}^k$ (eV)</th>
<th>$T_{max}^k$ (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>oxygen</td>
<td>O</td>
<td>0.308</td>
<td>20</td>
<td>130.3</td>
<td>148.5</td>
<td>32.0</td>
</tr>
<tr>
<td>copper</td>
<td>Cu</td>
<td>0.154</td>
<td>25</td>
<td>492.2</td>
<td>37.4</td>
<td>8.1</td>
</tr>
<tr>
<td>yttrium</td>
<td>Y</td>
<td>0.077</td>
<td>25</td>
<td>630.8</td>
<td>26.7</td>
<td>5.8</td>
</tr>
<tr>
<td>barium</td>
<td>Ba</td>
<td>0.154</td>
<td>25</td>
<td>856.9</td>
<td>17.3</td>
<td>3.7</td>
</tr>
</tbody>
</table>

* for $E = 662$ keV
§ for $E = 15$ MeV

that for electrons with energy 662 keV the Ba atoms have maximum kinetic energies lower than the corresponding threshold displacement energy. Then, for 662 keV electrons Ba displacements won’t be produced, and few will be expected for Cu and Y atoms due to the closeness of their $T_{max}$ values to the 25 eV horizontal line. Table 6.2 shows the $T_{max}$ values for each atom corresponding to minimum (662 keV) and maximum (15 MeV) electron kinetic energies in the studied range.

In figure 6.9, the dependence of the displacement cross sections on both displacement energy $T_d$ and electron kinetic energy $E$ for each atom are shown. Figure 6.9(a) illustrates how the displacement cross section depends on $T_d$ for incident energies of 662 keV and 15 MeV, which are the extremes of the studied energy range. As it can be observed, for 662 keV initial energy displacements for Ba atoms will not be produced for the selected $T_d$ values. The maximum kinetic energy of recoil atoms in this case (17.3 eV) is smaller than displacement energy (25 eV), see inset graph in figure 6.8 and Table 6.2. Very small amount of Y displacements will be produced for this initial energy, since recoiled Y atoms have a maximum energy of only 26.7 eV, too close to displacement energy value. When increasing initial energy both $T_{max}^k$ and $\sigma_d^k$ increase, and starting from $E = 1$ MeV dpa for all atoms will be produced ($T_{max}^{Ba} = 31.4$ eV is the smallest for this energy).

Figure 6.9(b) shows the dependence on the electron energy for the selected displacement energies, from which it is clear that increasing the incident energy the oxygen displacements appear first, later the Cu ones and afterwards the Y and Ba ones. This confirms the fact that for an incident energy of 662 keV no Ba atoms will be displaced and only a few of Y. From the inset of this figure one can see the energy for which displacement and PKA cross sections separate from each other, related to the beginning
of the displacement cascade processes. The corresponding electron kinetic energies are those exposed above.

Some additional comments about the McKinley-Feshbach approximation are necessary. As discussed in Section 2.4 it is assumed that this approximation is accurate to 1% for atomic number up to 40. Therefore, an error more than 1% should be expected only for Ba atoms ($Z=56$). But the PKA cross section for heavy atoms is usually much smaller than for light ones, and thus, the contribution from heavy atoms to the total dpa should be rather small. For this reason no significant error with the McKinley-Feshbach formula for YBCO is expected. This was justified by the calculations which are presented below.

For the dpa calculations the sample geometry was the same used in previous section. The irradiation conditions were also similar, $10^8$ photons impacted perpendicularly to the sample surface with initial energies from 662 keV to 15.0 MeV. The relative errors in all results were always below 5%.

Expression (4.5) is applied for all atoms in YBCO, taking into account their stoichiometry in the material. In this case the values for $T_d$ and $n_k$ in Table 6.2 are used. These results are shown in figure 6.10 for the selected $E_\gamma$ values. Also the displacement fluence in each voxel (Eq. (4.17)) was calculated from the energy fluence distributions obtained through MCNPX. These profiles appear in figure 6.11 to facilitate the comparison with
the corresponding dpa distributions, since the similarity in shape between them can be noticed. This will be discussed in the next Section 6.4.1.

The dpa values are always higher for larger incident energy in the whole volume of the sample. It is also interesting to note that the damage increases drastically with depth as the incident energy increases (increasing more than one order of magnitude in the sample thickness for \( E_\gamma \geq 3 \text{ MeV} \)). Besides, the maximum dpa damage moves deeper in the sample for higher incident energies.

From this calculation it is also possible to determine the contribution from each atom to the total dpa values. Averaging all dpa values throughout the sample thickness and volume, the total dpa value for each atom and incident energy can be obtained. The total values for each incident energy, taking together the contributions from oxygen and copper atoms (Cu-O\(_2\) plane), are shown in figure 6.12. It is easy to see that the contribution from the yttrium and barium atoms to the total are quite small in the studied energy range, therefore playing only a minor role in the changes of the material’s properties as stated by some authors [13,19]. Their contributions at high incident energy of 15 MeV are only of about 14% (Y) and 36% (Ba). Therefore, the biggest contribution to the total comes from the Cu-O\(_2\) planar sites, being >95% for low incident energies and also dominating at high energies with near 50% for 15 MeV.

The contribution from the oxygen and copper atoms inside the planes is also analyzed (figure 6.13). It can be easily observed that the contributions of both atoms also increase
with the incident energy. The oxygen atoms have a higher weight in the total dpa for all the studied incident energies. It is possible to see that for low energies the contribution comes essentially from the oxygen atoms, being more than 86% for energies \( \leq 1.25 \) MeV. However, as the energy of the incident photons increases, the contribution from the copper atoms also becomes important. Notice that for \( E_\gamma = 15.0 \) MeV the contribution from the copper atoms is about 48%. Then, it is necessary to keep in mind the copper atoms in this material at high energies and the possible effects that they could produce in material properties [59]. This result is consistent with evidences also observed previously by other authors [19,58].

### 6.4.1. Relation between dpa and energy deposition

Following the idea of the previous section, the energy deposition profiles for studied incident energies were also obtained through MCNPX. These profiles appear in figure 6.14. Lower energy radiation deposits more energy near the incident surface. However, moving deeper inside the sample higher energy deposition is found for more energetic incident radiation. The maximum energy deposition for each incident energy is found at deeper position when the incident gamma energy increases. Thus, for the last voxel in the incident direction, the energy deposition is higher for higher incident energy. This
is related to the nature of the energy deposition process. The energy deposition values involve the total energy deposited by all photons and electrons in a given volume. For higher incident gamma energies more interaction processes become available and the interaction depth increases, increasing also the number of secondary particles generated.

Figure 6.14.: In-depth energy deposition profiles in YBCO for different incident gamma energies.

Figure 6.15.: Dependence between dpa and energy deposition for different incident gamma energies.

Figure 6.16.: Displacements per atom to energy deposition ratios for different incident gamma energies.
Comparing the dpa distributions from figure 6.10 with these energy deposition profiles some similarity in shape can be observed. As in previous section figure 6.15 shows the possible dependence between them. Large correlations among dpa and energy deposition are obtained for all incident energies, with Spearman coefficients from 0.93 to 1.00 (significant at the 95%). However, the dependence between dpa and energy deposition shows a deviation from the linearity for incident energies higher than 3 MeV, with more dispersion for higher energy deposition values. This is related with the previous discussion.

Finally, the dpa to energy deposition production ratios are calculated by taking the total dpa and energy deposition values for each incident energy (figure 6.16). Here one can see that the gamma radiation energy deposition mechanism increases the probability for atom displacements at higher incident energies.

6.5. Study of positrons contribution to dpa profiles

At low gamma energy irradiation only electrons play a role in dpa formation. But with increasing energy of the gamma irradiation, electron-positron pair production becomes important and therefore the role of the positrons in producing atom displacements also increases significantly. A first attempt of evaluating the positron contribution to the dpa distribution was reported by Cahn for Si and Ge [4] and more recently by Fukuya and Kimura for Fe [54]. They used theoretical expressions for the different gamma-material interaction processes as discussed in previous chapter. In this section the MCCM calculation procedure introduced in Chapter 4 is applied to evaluate the positron contribution to the total dpa values in the YBCO.

Figure 6.17(a) shows the displacement cross section for electrons and positrons for each atom in YBCO. It is observed that the displacement cross section for positrons is lower than for electrons, although both present a similar behavior with energy. For better comparison, the ratio of electron to positron displacement cross section for each atom, \( \frac{\sigma_d^k(e^-)}{\sigma_d^k(e^+)} \), is presented in figure 6.17(b). This ratio between both cross sections is higher for heavier elements, reaching a maximum from only about 1.11 for oxygen atoms up to near 2.83 for barium ones. That difference increases rapidly for lower electron/positron energies, obtaining the maximum within 0.7 MeV and 1.6 MeV for all four atoms. For higher energies the positron cross section increases faster than the electron one, being only about 1.05 and 1.70 times lower.
Figure 6.17.: (a) Displacement cross sections for electrons (continuous lines) and positrons (dashed lines) and (b) electron to positron displacement cross section ratios for all atoms in YBCO.

Figure 6.18.: In-depth dpa distributions produced by (a) electrons and (b) positrons in YBCO for different gamma irradiation energies.
An identical sample geometry was used as in previous sections and similar simulation conditions were defined. The energy range is selected in this case from 1 MeV up to 15 MeV. Each one of the four atoms that constitutes the material is also taken into consideration. With the help of the MCNPX simulation code, the energy distribution of electron and positron fluences are determined separately. Then the number of displacement per atom is calculated through the MCCM procedure taking for $T_d$ and $n_k$ the same values reported in Table 6.2. The results of electron and positron contributions to the total number of displacements versus the sample depth are shown in figure 6.18.

First, it is important to remark that the shape of the positron profiles are very similar to those of the electrons: dpa values are always higher at higher incident radiation energies in all the sample volume, and the damage increases drastically with depth as the incident energy increases. For 1 MeV incident gamma energy only displacements by electrons will be present, since there is no production of positrons for energies lower than 1.022 MeV ($2mc^2$). It is observed that for lower gamma energies the electron contribution is much higher than the positron one, being about two order of magnitude higher for 2 MeV incident energy. As the gamma energy increases that difference becomes smaller and the positrons induced dpa values are about the half that of electrons dpa values for 15 MeV.

It is better noticed by analyzing the total dpa for each $E_\gamma$, considering the contributions from electrons and positrons. The total dpa values due to electrons and positrons for different gamma energies are presented in figure 6.19. Also, the electron and positron partial contributions are shown as percentage bars. From this figure it can be seen that electrons have a larger contribution to the total dpa for all the studied gamma irradiation energies. For higher irradiation energies the difference between them is reduced. The positrons contribute for 32% of the total dpa at $E_\gamma = 15$ MeV, almost the half than the corresponding contribution induced by electrons. Then when positrons are considered the total dpa increases, being about 47% higher that if were not considered for 15 MeV gamma irradiation.

As stated in previous chapter, some authors do not considered positrons at all [3,104]; some others treat positrons as electrons [101,146]. Positrons are neglected considering they have a short live since they annihilate fast with surrounding electrons. However the positrons interaction cross section for elastic processes is 5-6 orders of magnitude higher than the corresponding annihilation cross section in the studied energy range. In addition, the positrons mean free path for annihilation process is 6-7 orders of magnitude higher than for elastic process. This indicates that positrons will have several elastic
interactions before annihilation. Besides, positrons with 1 MeV kinetic energy have a range about 1.3 mm, which represents about $10^8$ times the YBCO unit cell parameter. Thus, positrons should not be neglected in this kind of studies, as it is supported by the results presented below.

In figure 6.20 the influence of possible positron treatment in this kind of studies is then analyzed: (1) positrons and electrons are both considered, (2) positrons are considered as electrons and (3) positrons are neglected. The results considering both electrons and positrons give dpa values up to 1.14 times lower than the case of considering positrons as electrons. When positrons are neglected the dpa values decrease up to 1.47 times with respect to the case of considering both electrons and positrons. The energy dependence of the total dpa is the most gentle for the approximation neglecting positron contribution since the pair production process becomes more important for higher incident gamma energies. In this way, the influence of positron treatment for dpa calculations in gamma radiation damage studies is systematically studied for the first time.

The contribution from each atom to the total dpa value is also studied through figure 6.21. As in previous section the contribution of the Cu-O$_2$ plane is considered. The results show that, when positrons are considered, the contribution to the total damage from yttrium and barium atoms is also smaller than the contribution from the Cu-O$_2$
planes. They have a maximum contribution of only about 14% (Y) and 33% (Ba) for 15 MeV of incident radiation. The main contribution to the total damage comes from the Cu-O$_2$ planar sites. Figure 6.21(a) shows that the in-plane dpa contribution is about 53% of the total dpa in the sample for 15 MeV incident gamma radiation, being much higher for lower incident energies. All this leads to total in-plane dpa up to about 1.6 times higher when considering positrons respect to the case when they are not taken into account.

The independent contributions from oxygen and copper atoms to the in-plane dpa are shown in figure 6.21(b). From this figure it is possible to observe that the contribution from oxygen atoms dominates over the Cu one for all studied energies. Making some evaluation it is noticed that considering positrons in the calculation increases the contribution from oxygen atoms to the in-plane dpa in about 4%. However, the O-dpa values diminish with increasing the incident energy while the contribution from Cu-dpa increases. The main dpa contribution with regard to the Cu-O$_2$ planes arises from O-displacements, being about 93% for 1 MeV of gamma irradiation. At higher gamma energies, an increasing role of Cu-displacements is observed, reaching about 46% of the in-plane dpa for 15 MeV incident energy.

![Figure 6.21](image.png)

**Figure 6.21.** Contributions (a) from Cu-O$_2$ planes and Y and Ba atoms to total dpa in YBCO and (b) from oxygen and copper atoms to dpa inside planar sites.
6.5.1. Dpa to energy deposition ratio

Following the idea of the previous sections, the dependence between dpa distributions and energy deposition profiles are also analyzed. Figure 6.22 shows the dpa to energy deposition ratios for different incident gamma energies. The case where positrons are considered as electrons is also included. Again, when the positrons are considered as electrons, an overestimation in the result is obtained. In that case the dpa production ratio is about 1.10-1.14 times higher than when positrons are considered together with electrons. Again, this is a clear indication that the treatment of positrons in dpa calculation influences the final result.

Figure 6.22.: Displacements per atom to energy deposition ratios for different incident gamma energies.

6.6. Dpa profiles in YBCO irradiated with electrons

It is well-known that the main dpa formation process is due to elastic scattering events of energetic charged particles (electrons and positrons) with atomic nuclei. Irradiation with electrons could be more efficient than gamma irradiation in producing dpa by interacting directly with atomic nuclei. Electron irradiation is a technique widely used to produce different defects in HTSs [19,198,208,209].
In the present section the effects of electron irradiation on YBCO dpa profiles is studied. For this purpose, the same sample and simulation conditions from previous sections are used. The electron incident kinetic energy $E_0$ is varied from 1.0 MeV to 10.0 MeV in intervals of 1.0 MeV. Values for $n_k$ and $T_d$ are also the same.

Following the MCCM procedure, the numbers of displacements per atom is calculated for all atoms in YBCO. These results are shown in figure 6.23, representing the in-depth dpa distributions for different electron irradiation energies.

The dpa values are always higher for higher incident radiation energy in the whole sample volume. It is interesting to note the difference with the case of gamma irradiation. In that case dpa values are increasing with depth in the sample, even more drastically as the incident energy increases (figure 6.18). In fact, gamma irradiation dpa profiles showed a strong depth dependency at higher energies. In contrast, for electron irradiation the behavior is different. At lower energies, the dpa profile has a maximum near to the incident surface and then decreases quickly with depth. When increasing the incident
energy the distribution maximum moves to a deeper position inside the sample. After reaching a maximum the dpa values decrease fast reaching values at the outgoing surface that are lower than at the incident surface. For energies higher than 8 MeV dpa profiles become smoother and monotonously decreasing. This indicates that dpa’s are more homogeneously distributed in depth at higher electron irradiation energies. This is a significant difference with the gamma irradiation effect previously observed. Furthermore, dpa values produced by electron irradiation is about three order of magnitude higher than dpa values in the case of gamma irradiation. This way the electron irradiation is more effective in provoking dpa damage inside the material than the gamma irradiation.

Figure 6.24 presents the in-depth energy deposition profiles for different electron irradiation energies. These profiles will be discussed later in the next subsection, but they are presented here for better comparison with the corresponding dpa distributions in figure 6.23.

The total dpa values over the sample thickness for each energy is calculated, in such a way that the contributions from secondary electrons and positrons could be evaluated separately. The differences between the electron and positron partial dpa contributions are shown in figure 6.25. As can be seen from this figure, dpa produced by electrons have a greater contribution to the total dpa in all the studied energy range. The positron dpa contribution is too small with respect to dpa induced by electrons (5-7 orders of magnitude lower).

![Figure 6.25: Dpa induced by electrons and positrons in YBCO at different electron irradiation energies.](image-url)
magnitude lower). This is an important difference with respect to the case of gamma irradiation, where the positron dpa value at 10 MeV is about 37% of the electron dpa value (figure 6.19). Another difference is that in this case positrons produce dpa for incident electron energies higher than 3 MeV. This is related with the fact that positrons are produced in this case through the secondary photons pair production processes, which present low interaction cross section for lower photon energies. Those secondary photons are produced by electrons brake radiation, also with lower interaction cross section, about 4-5 order of magnitude lower than elastic and inelastic events.

The contribution from each atom to the total dpa value is also studied. The results show that the contribution to the total dpa from yttrium and barium atoms is smaller than the contribution from the Cu-O$_2$ planar sites for all studied energies. Y and Ba have a maximum contribution, related to the total, about 15% and 38% respectively for 10 MeV of incident radiation (figure 6.26). These contributions are slightly higher than for the case of gamma irradiation (14% for Y and 33% for Ba).

The independent contributions from oxygen and copper atoms to the total in-plane dpa are shown in figure 6.27. In this figure one can observe that the contribution from oxygen atoms diminishes by increasing the incident energy while the contribution from copper atoms increases. The O-dpa dominates over Cu-dpa for energies up to 7 MeV, 

**Figure 6.26.** Displacements from Y and Ba atoms and from the Cu-O$_2$ planar site.

**Figure 6.27.** Contribution from oxygen and copper atoms to total in-plane dpa.
when displacements of copper become higher, representing about 51% for 10 MeV incident electrons.

There is a remarkable difference with the gamma irradiation results, where the Cu-dpa produced are always lower than oxygen ones for all studied incident energies. For 10 MeV gamma irradiation Cu-dpa are about 12% lower than O-dpa. These results indicate that electron irradiation is also more effective displacing copper atoms inside the planar sites in YBCO that the gamma irradiation.

### 6.6.1. Displacements per atom and energy deposition

The dependences between dpa distributions (figure 6.23) and energy deposition profiles (figure 6.24) are also analyzed. The relative good similarity in shape of respective profiles for incident energies up to 3 MeV can be observed. For higher incident energies the difference among dpa and $E_{dep}$ distributions increases, being them completely different for $E_0 > 7$ MeV. This is confirmed by the Spearman coefficients, giving large correlations about 0.64-0.98 (95% significant level) for incident energies up to 3 MeV. Correlations for energies 4-7 MeV are acceptable, with values about 0.56-0.42, but they are small for higher incident energies. The displacements per atom to energy deposition ratios are then estimated by evaluating their total values for each incident energy.

![Figure 6.28.](image.png)

**Figure 6.28.** Dpa to energy deposition ratios for different electron and gamma irradiation energies.
Figure 6.28 shows the dpa to energy deposition ratio for different electron irradiation energies, together with those previously calculated for incident gamma rays. It can be observed that this ratio increases for higher incident electron energies. This behavior is similar to the case of gamma irradiation studied in previous sections. But irradiating with electrons leads to ratio values that are twice the corresponding values in the case of gamma irradiation for lower irradiation energies. For higher incident electron energies the dpa to energy deposition ratio increases fast. For 10 MeV electron irradiation energy it is about 17 times higher than the corresponding value for incident gamma radiation.

6.7. Chapter conclusions

First, the oxygen displacements in chain and plane crystalline sites at low gamma irradiation energies were analyzed. The contribution from the $O_c$ atoms to the total calculated dpa value dominates in the whole studied volume, with about 80% for 1.25 MeV photon irradiation. This contribution is $\sim 86\%$ and 100% in the case of 662 keV and 122 keV incident photons respectively.

The results for higher incident gamma energies showed that the dpa damage increases drastically with depth, even more than one order of magnitude in the sample thickness for $E_\gamma \geq 3$ MeV. The contributions from the Y and Ba atoms to the total dpa were quite small for the studied energies. The O-dpa values dominate for all the incident energies. However, as the incident photons energy increases, the contribution from the Cu atoms becomes important, being about 48% for $E_\gamma = 15.0$ MeV.

The positron treatment for dpa calculations in gamma radiation damage studies was found to be important. The positron contribution is small for low incident energy and increases with this last one. When positrons were considered in the calculation, the total dpa increases in about 47% for 15 MeV gamma irradiation. The results considering both electrons and positrons gave dpa values up to 1.14 times lower than the case of considering positrons as electrons. When positrons were neglected the dpa values decreased up to 1.47 times on regard to considering both electrons and positrons.

In contrast with the case of gamma irradiation, the behavior of electron irradiation induced dpa is quite different. At higher energies dpa profiles become smoother and monotonously decreasing. This indicates that dpa values distribute more homogeneous in depth at higher electron irradiation energies. The dpa values produced by electron
irradiation were about three order of magnitude higher than the dpa values induced by the gamma irradiation. This way the electron irradiation was more effective in provoking dpa damage inside the material than the gamma irradiation. The results indicated that electron irradiation is also more effective displacing copper atoms inside the planar sites in YBCO that the gamma irradiation. The O-dpa dominates for incident electron energies up to 7 MeV, when displacements of copper become higher. This is a remarkable difference with the gamma irradiation results, where the O-dpa values are always higher than copper ones for all studied incident energies.

Last, based on the good correlation found between the dpa and energy deposition profiles for each incident energy, it was possible to evaluate the dpa to energy deposition ratio. It was found that the gamma radiation energy deposition process in YBCO material supports better the atom displacement production at higher incident energies. Irradiating with electrons gave a dpa to energy deposition ratio that doubles the corresponding in the case of gamma irradiation for low irradiation energies, and was about 17 times higher for 10 MeV irradiation energy.
Chapter 7.

Radiation damage evaluation on LYSO and LuYAP crystals

“The most exciting phrase to hear in science,
the one that heralds the most discoveries,
is not “Eureka!” but “That’s funny…””
— Isaac Asimov (1920–1992)


7.1. Introduction

The study of the radiation detectors is a never-ending field in experimental nuclear physics, determined not only by the constant growing applications, but for the permanent development of new materials with more advanced properties. One of the most important application of radiation detectors is found in medical physics. Our research group has been working on the research and development of semiconducting and scintillating detectors, mainly for medical imaging applications, such as mammography, computed tomography and particle emission tomographies.
Positron Emission Tomography (PET) is nowadays one of the more studied systems due to its present and future importance in diagnostic medical imaging. The ClearPET® system [210] (figure 7.1) is a second generation high performance PET scanner first combining high resolution and high sensitivity by using new technologies in crystals and electronics. The novelty of this system is that the detection head is composed of double layer small scintillating crystals: lutetium-yttrium oxyorthosilicate (Lu$_{1.8}$Y$_{0.2}$SiO$_5$ or LYSO) and lutetium-yttrium orthoaluminate (Lu$_{0.7}$Y$_{0.3}$AlO$_3$ or LuYAP). These crystals are arranged in phoswich (phosphor sandwich) configuration in order to improve the depth of interaction for better radial resolution.

LYSO and LuYAP seem to be a compromise between fast response and relatively high light yield. These crystals offer high density, high light output, good energy resolution and short decay time that make them ideal in a wide range of gamma ray detection applications [211–213]. Exposure of high-energy radiation on these materials generally produce various interesting changes in their properties, which include physical, chemical, electrical, magnetic, mechanical as well as optical properties [214–220]. These radiations mainly produce ionization and displacement in the constituent elements of the samples. Ionization effects disappear fast in the case of good conductors and produce heating in the materials, whereas in insulators, electrons produced by ionization get trapped in the lattice imperfections producing permanent changes in the material. Not any work related to the study or estimation of the dpa damage produced by gamma radiation on these crystals was found before the contribution made in this thesis.

In this chapter the radiation damage in dpa terms induced in LYSO and LuYAP crystals by gamma irradiation and gamma induced secondary electrons generated is studied. As gamma sources for this study we use $^{44}$Sc (1.157 MeV maximum peak), $^{22}$Na (1.275 MeV maximum peak) and $^{48}$V (0.984 and 1.312 MeV maximum peaks). These sources are typically $\beta^+$ emitters, but the emitted positrons are quickly annihilated. Then, the energy of gammas from the e$^-$e$^+$ annihilation processes (511 keV) is also included in the study as gamma source. This procedure allowed studying the in-depth dpa distributions inside each crystal for all four sources. It is also possible to obtain the separate contribution from each atom to the total dpa.
Figure 7.1.: ClearPET® structure showing PMT detector cassette and crystals block.

Figure 7.2.: Geometry, dimensions and properties of the model used for simulation.
7.2. Model for Monte Carlo simulation

The geometry and properties of the simulated model can be observed in figure 7.2, focusing the attention on the dual layer scintillating phoswich matrices, consisting of $8 \times 8$ LYSO and $8 \times 8$ LuYAP crystals block elements. Each crystal element has dimension of $2.0 \, \text{mm} \times 2.0 \, \text{mm} \times 10.0 \, \text{mm}$. A thin BaSO$_4$ layer (0.3 mm width) separates the LYSO and LuYAP crystals, as in the experimental arrangement.

The irradiation process is simulated with $10^8$ photons impacting isotropically on the exposed surface of the LYSO crystals. In separate simulations the incident photon energy $E_\gamma$ is selected considering each one of the studied sources, taken their full gamma spectra disregarding the $e^-e^+$ annihilation contribution, which is considered by including another source of photons with 511 keV energy. For the calculation of in-depth dpa profiles each crystal is divided in 10 voxels with 1.0 mm length. All the simulation results have relative errors below 5%.

7.3. Threshold displacement energies

Displacement energies for LYSO and LuYAP materials are not reported in literature. Jacobsohn and coworkers studied the role of oxygen on proton-irradiated Lu$_2$SiO$_5$ (LSO) luminescence [221]. They used 25 eV, 15 eV and 28 eV as displacement energies for Lu, Si and O atoms respectively in order to estimate the vacancy concentrations in LSO. Another previous work reported threshold displacement energies in pure Si material with average values of 14.7 eV and 17.5 eV calculated by molecular dynamics for two different approximations [82]. On the other hand, different experimental and calculated threshold displacement energies for Al in Al$_2$O$_3$ ceramics have been reported in the range 18-32 eV [76, and references therein]. But the recommended value in that review (averaged over the low-index crystal orientations) is $\sim 20$ eV. This is supported by a recent study on molecular-dynamics simulation of threshold displacement energies in lithium aluminate (LiAlO$_2$) [86]. Averaging their results for Al over the low-index crystal orientations, $T_d \sim 21$ eV.

Taking into account the above findings, the following values for the displacement energy have been selected for our calculations, independently of the crystal: 28 eV for O atoms, 20 eV for Al, 15 eV for Si and 25 eV for Y and Lu atoms.
7.4. Displacement cross section

The calculated displacement cross sections for each atom in both crystals is shown in figure 7.3. It is possible to identify $E_c$ values in the region up to $\sim$1 MeV for each atom. Photons from annihilation processes could not produce displacement of Y and Lu atoms. The electron energies for which the dpa cascade processes begin are indicated in this figure by arrows. Multiple displacements then occur for electron kinetic energies higher than about 299 keV for Si atoms, 314 keV for O atoms, 365 keV for Al, 1.02 MeV for Y and 1.58 MeV for Lu. It is clear that dpa cascade events for Lu atoms will almost never occur with the studied gamma sources.

An error more than 1% should be expected in the evaluation of the displacement cross section for Lu atoms ($Z=71$) through the McKinley-Feshbach approximation. But no significant error in the dpa calculation are expected for these materials, since the Lu atom is much heavier than the rest and its contribution should be small.

7.5. Calculation of dpa distributions

Applying the MCCM procedure, the number of displacement per atom is evaluated. First the total dpa value in each one of the 64 crystals of LYSO and LuYAP, in order to evaluate the spatial distribution of the dpa damage in the crystals array, is calculated. As example, figure 7.4 shows these results in LYSO for each one of the studied gamma sources. The dpa damage accumulates more in the central crystals, being higher in about 88-91% than in the border ones. The results in LuYAP are similar. This result is related to the contribution that each crystal receives from secondary electrons coming from neighbor crystals. Thus, as border and corner crystals have smaller quantity of neighbors than the rest, they will result in lower dpa values. This result is possible to achieve in the frame of the proposed methodology, through the Monte Carlo simulation of radiation transport in the material. With the previous theoretical calculations it was not possible to consider this effect.

The total dpa values in the LYSO and LuYAP crystal matrices are now considered by averaging all crystal values in each case for all studied gamma sources, as is shown in figure 7.5(a). The first conclusion that can be drawn is that dpa produced by photons coming from annihilation processes is an important contribution when compared to the other sources. Displacements produced by 511 keV photons in LYSO crystals is about...
Figure 7.3.: Displacement cross section for all atoms in LYSO and LuYAP crystals. Arrows indicate the energy value where the cascade processes start. $E_c$ values are shown between parenthesis.

Figure 7.4.: Mapping distribution of total dpa induced in 8×8 LYSO crystals array by each one of the studied sources.

77%, 71% and 39% of the dpa created by the $^{44}$Sc, $^{22}$Na and $^{48}$V sources respectively. In the LuYAP crystals that proportion is smaller but still important, being correspondingly 52%, 46% and 22%.

Also, figure 7.5(a) shows that dpa damage in LYSO crystals is higher than in LuYAP crystals, decreasing the difference between them when more energetic sources are used. Irradiation with 511 keV photons produces a total dpa on LYSO crystals about 16 times higher than on LuYAP ones, while for the $^{48}$V gamma source this ratio is about 9. The
Radiation damage evaluation on LYSO and LuYAP crystals

Figure 7.5: Total dpa produced by each gamma source in LYSO and LuYAP crystal matrices (a) in the original configuration and (b) interchanging LYSO and LuYAP positions.

dpa radiation damage generated in LuYAP crystals is about 6-11% of the corresponding one in LYSO crystals for the analyzed sources. This is directly related to gamma and electron energy loses as the radiation penetrates in the detector. Photons with lower energy produce low energy electrons, which decreases the probability and efficiency of atom displacements formation processes.

In order to make a more suitable comparison between LYSO and LuYAP radiation exposure in terms of dpa, their positions are interchanged and the calculations are repeated. Now, LuYAP crystals receive directly the photons from the sources. The corresponding results are presented in figure 7.5(b). In this case the dpa values in LuYAP crystals are higher than in LYSO crystals, as expected from the previous analysis. But the difference between them is lower than in the former case, being the dpa values on LYSO crystals about 11-15% with respect to the corresponding one on LuYAP crystals for the studied sources. This is mainly related to the displacements cross section values for Si and Al atoms, which are the basic difference in both materials. Displacements cross section for Si is higher than for Al for the selected displacement energies (figure 7.3). In the phoswich configuration, the secondary electrons kinetic energy in the first layer will be higher than in the second layer, when it is irradiated by gamma radiation. Then, the difference between the displacement cross section values for Si and Al atoms in configuration (a) is higher than in configuration (b), i.e., $\sigma_d^{Si}(E_2) - \sigma_d^{Al}(E_1) > \sigma_d^{Al}(E_2) - \sigma_d^{Si}(E_1)$ for $E_2 > E_1$. 
Comparing now each crystals layer in phoswich configuration (a) with its corresponding in configuration (b), LYSO and LuYAP can be compared under the same irradiation conditions. The displacements induced by 511 keV photons on LuYAP crystals (in configuration (b)) are about 79% of those ones on LYSO (in configuration (a)). When they are located in the second crystals layer, the dpa values in LuYAP (a) are about 70% of dpa values in LYSO (b). This ratio (LuYAP to LYSO dpa) is about 84% (in the first layer) and 81% (second layer) for the dpa produced by $^{44}\text{Sc}$ and $^{22}\text{Na}$ sources. $^{48}\text{V}$ sources produce displacement damage on LuYAP crystals that is about 87% (first layer) and 85% (second layer) of the corresponding values for the LYSO crystals. It can be then concluded that LuYAP crystals gathered lower dpa values than LYSO crystals.

The total dpa damage in the phoswich detector is now taken as the average of the displacements on LYSO and LuYAP crystals. Thus, the dpa damage generated in the crystals block for the configuration (b) is about 83-90% lower than in case (a). Interchanging the LYSO and LuYAP layers in the detector block the dpa damage reduces about 17% for 511 keV incident photons and about 10% for $^{48}\text{V}$ gamma source.

Typical gamma sources for PET studies have an activity about 1 mCi. Considering this, our results give a dpa rate of about $1.5 \cdot 10^{-19}$ to $4.4 \cdot 10^{-19}$ dpa/s for the studied gamma sources. This is a low dpa damage rate, meaning that the LYSO and LuYAP crystals present a low exposure to the gamma radiation damage.

The possibility of substituting LYSO and LuYAP crystals by the CZT semiconductor material has been investigated in this thesis as well. Simulations for this configuration (figure 7.2) were executed, substituting LYSO and LuYAP by CZT, and the dpa total values induced in the detector block are calculated. Results are presented in figure 7.6 together with results from previous configurations (a) and (b) for LYSO and LuYAP crystals. One can see that produced displacements are higher in CZT material than in LYSO and LuYAP configurations for all studied gamma sources. The dpa damage in CZT is about 1.4 to 5.6 times the obtained in the LYSO-LuYAP configuration and 1.7 to 6.3 times the corresponding in the LuYAP-LYSO case, considering the studied sources. This is related to lower values of the displacement energies for atoms in CZT, resulting in higher displacements cross sections. Thus, LuYAP-LYSO configuration are characterized by the lowest exposure to dpa damage induced by the gamma sources here considered.

Now, the separate contributions from each atom in both LYSO and LuYAP crystals are discussed. The contributions from each atom to the total dpa values presented in figure 7.5(a) are also estimated and they are showed in figure 7.7.
Figure 7.6.: Total dpa produced by each gamma source in the whole detector block of CZT. Results with configurations (a) and (b) for LYSO and LuYAP crystals are also included for comparison.

Figure 7.7.: Individual contributions from each atom to the total dpa induced by different gamma sources.

Figure 7.8.: Total dpa in-depth profiles induced in LYSO and LuYAP crystals by each studied source. Gray line represents the BaSO$_4$ layer.
First, contribution from Y and Lu atoms to the total dpa can be neglected in all the cases (always below 1%). Even, they are not produced at all by photons coming from 511 keV source. The oxygen displacements dominate in both crystals for all gamma sources. In LYSO crystals O-dpa values contribute with 57 to 58% to the total dpa for the studied sources. Si-dpa values induced by the same sources then represent 43 to 41% from the total dpa in the same crystals. In the case of LuYAP crystals, the O-dpa values dominate with a contribution of about 67% (for 511 keV photons) to 61% (for $^{48}$V source) relative to the total dpa. Al atom displacements increase with source energy, from about 33% for 511 keV photons to 37% for $^{48}$V source relative to the total dpa in these crystals.

For studying the in-depth dpa profiles, one crystal located near the center of the crystals matrix, for both LYSO and LuYAP, is selected. Figure 7.8 shows the dpa distribution’s evolution with depth in both crystals for each used gamma source. The dpa damage is maximal close to the LYSO photons impacted surface, since dpa values for all sources decrease with depth inside the detector. This behavior is stronger for 511 keV photons, where dpa values diminish by about 99% in the full phoswich depth (94% in the LYSO crystal and 78% inside the LuYAP crystal). This reduction is somewhat smaller for the other sources being $\sim$91-92% inside the LYSO crystal and $\sim$73-74% inside the LuYAP crystal ($\sim$98% in the full detector length).

### 7.6. Displacements to energy deposition ratio

The energy deposition profiles in LYSO and LuYAP crystals are also obtained through MCNPX for the gamma sources under discussion. As in previous chapter, in-depth dpa distributions and energy deposition profiles produced by each source are compared, as presented in figure 7.9 for both crystals. LYSO in configuration LYSO-LuYAP and LuYAP in configuration LuYAP-LYSO are considered in order to compare them. The Spearman correlation coefficients between dpa and energy deposition for all studied sources in both crystals give values of 1.0. Besides, the nearly linear dependence between them for all studied sources is observed, since low energy sources are studied.

Following the same idea from previous chapter, the dpa to energy deposition ratio can be estimated by fitting their dependencies from figure 7.9. Table 7.1 presents these results for both crystals and the four analyzed gamma sources. As obtained for previous studied materials, dpa to $E_{dep}$ ratio increases for more energetic photon sources. This ratio is 1.22 times higher in LYSO than in LuYAP crystals when they are irradiated by
Radiation damage evaluation on LYSO and LuYAP crystals

511 keV photons. This difference is slightly lower for the other sources, being 1.13 times for $^{44}$Sc, 1.14 for $^{22}$Na and 1.09 times for irradiation with $^{48}$V gamma source.

Figure 7.9.: Dependence between dpa and energy deposition by different gamma sources in LYSO and LuYAP crystals. Continuous lines represent the linear fitting.

Table 7.1.: Dpa to energy deposition ratios in LYSO and LuYAP crystals for all studied gamma sources. Fitting adjusted R-Squares are also presented.

<table>
<thead>
<tr>
<th>$\gamma$ source</th>
<th>LYSO</th>
<th>LuYAP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\eta \pm \Delta\eta$ (10$^{-24}$ dpa/MeV) &amp; Adj. R-Square</td>
<td>$\eta \pm \Delta\eta$ (10$^{-24}$ dpa/MeV) &amp; Adj. R-Square</td>
</tr>
<tr>
<td>511 keV</td>
<td>4.525 ± 0.054 &amp; 0.999</td>
<td>3.724 ± 0.045 &amp; 0.999</td>
</tr>
<tr>
<td>$^{44}$Sc</td>
<td>6.335 ± 0.083 &amp; 0.998</td>
<td>5.614 ± 0.054 &amp; 0.999</td>
</tr>
<tr>
<td>$^{22}$Na</td>
<td>6.728 ± 0.075 &amp; 0.999</td>
<td>5.908 ± 0.073 &amp; 0.998</td>
</tr>
<tr>
<td>$^{48}$V</td>
<td>11.325 ± 0.096 &amp; 0.999</td>
<td>10.379 ± 0.100 &amp; 0.999</td>
</tr>
</tbody>
</table>
The radiation damage in dpa terms induced by different gamma sources irradiation in LYSO and LuYAP crystals was studied in this chapter.

The total dpa produced by photons coming from electron-positron annihilation processes is an important contribution relative to the $^{44}$Sc (75%), $^{22}$Na (69%) and $^{48}$V (37%) sources. It was observed that for the LuYAP crystals that proportion is slower, but yet important.

The dpa damage in LYSO crystals was higher than in LuYAP crystals, but the difference between dpa produced in LYSO and LuYAP decreased when more energetic sources were used. Interchanging the positions of LYSO and LuYAP crystals block inside the phoswich a more suitable comparison between them was possible. The results allowed to conclude that the LuYAP crystals get a lower dpa exposure than the LYSO crystals. The total dpa damage in the whole detector crystals block (LYSO + LuYAP) for the LuYAP-LYSO configuration was lower than for the LYSO-LuYAP case for all the studied sources.

The contributions from Y and Lu atoms to the total dpa were below 1% and can be neglected in all cases. In contrast, the oxygen displacements dominate in both crystals for all gamma sources.

The atom displacement damage is maximum close to the photons incident LYSO surface, since the dpa values for all sources decrease with depth inside the detector. This behavior was stronger for 511 keV incident photons, despite its dpa values diminished by about 94% in the LYSO crystal and 78% in the LuYAP crystal. This reduction is somehow smaller for the other sources being ~91-92% inside the LYSO crystal and ~73-74% inside the LuYAP crystal length.

The correlation between dpa and energy deposition profiles was excellent and their ratio was found to increases with more energetic photon sources. LYSO crystals are more liable to the dpa damage than LuYAP crystals. The displacement to energy deposition ratio was between 1.22 (for 511 keV incident photons) and 1.09 (for $^{48}$V source) times higher in LYSO than in LuYAP crystals.
Chapter 8.

Displacement damage by gamma rays in a CZT matrix detector

“But in science the credit goes to the man who convinces the world, not to the man to whom the idea first occurs.”
— Sir Francis Darwin (1848–1925)

This chapter is related with the paper: Radiation damage study in CZT matrix detectors exposed to gamma rays, A. Leyva, I. Piñera, O. Dona, A. Díaz, C. M. Cruz, Y. Abreu, L. M. Montaño, Nucleus 45 (2009) 32–36.

8.1. Introduction

Since the early 1990’s the detection properties of semiconductor detectors have been drastically improved with the introduction of new materials like cadmium zinc telluride (Cd$_{1-x}$Zn$_x$Te or CZT). This compound is based on the well known cadmium telluride (CdTe), replacing a fraction of Cd by Zn, increasing this way the resistivity and decreasing the leakage current of the detectors. Good detection efficiency and high energy-resolution make CZT and CdTe attractive in many room temperature gamma and X-rays applications such as industrial and medical imaging [222], as for example: digital mammography and angiography or PET [223,224]. In the last decade the use of CZT in fabrication of semiconductor radiation detectors has undergone an important technological step [225]. Many researchers have proposed the use of pixelated semiconductor detectors made
from CZT or CdTe as a strategy to improve the spatial resolution of nuclear medicine systems [226–230].

In this chapter some aspects of gamma radiation damage in room temperature CZT detectors for imaging applications are analyzed. There are two main effects on semiconductor devices: the transient effect, which is used to measure the dose rate, and the displacement effect, which causes damage. The initially produced defects from gamma irradiation can be expressed as a single displaced lattice atom and its associated vacancy [231,232]. These Frenkel defects are related with the degradation in the minority carrier lifetime or diffusion length in the base region. Thus, displacement effects on semiconductors are considered to be quite important [233].

In this sense, a novel configuration of PET systems is studied. It consists of an experimental variant allowing to detect a third photon from the source, in order to improve the spatial resolution of the system [234,235]. This photon is first sensed by a position sensitive CZT semiconductor detector where it undergoes Compton scattering and then is later detected by scintillating external detectors. This Compton detector is designed as a ring of detecting units, introduced inside the classical scintillating ring of the PET system, like it is shown in figure 8.1.

8.2. System model for calculations

Figure 8.1 shows schematically the basic detecting geometry typically employed in small animal PET imaging systems used for research. In this case, a Compton detector ring is included between the studied body and the scintillators ring. The analysis is focused on one of the 24×24 pixels CZT matrix detectors (5 mm thickness) with gold electrodes. Each pixel is 280 µm × 280 µm. This detector is isotropically irradiated by a point radiation source placed inside a water octahedron, which simulates a mammal body. Two different point sources emitting photons were selected for simulation: a commonly used $^{22}$Na source (maximum photons peak at 1.275 MeV) and photons coming from electron-positron annihilation (511 keV). For the calculation of in-depth profiles, the central pixel of the matrix is selected, subdividing it in 25 voxels with 200 µm length.

All the geometrical and physical details of the system, as well as constituent material properties are taken into account in the simulation. All results have a relative error below 5%, which is guaranteed using $10^8$ source photons in each simulation experiment.
8.3. Threshold displacement energies in CZT

Displacement energies for atoms in CZT material are not explicitly reported in literature. But some authors consider that strictly speaking CZT is an alloy of binary compounds CdTe and ZnTe. Bryant and coworkers have studied these compounds and have estimated their displacement energy values [236–240]. They first studied the luminescence emission spectrum of cadmium telluride before and after bombardment with low monoenergetic electrons [236,238]. They found threshold energies for the production of primary damage in the crystal at 235 keV and 340 keV for Cd and Te atoms respectively. Electrons with those energies could transfer a maximum of 5.6 eV to a cadmium atom and 7.8 eV to a tellurium atom. In later investigations the effect of lattice damage by energetic electrons on zinc telluride was monitored by Meese [241] and Bryant and Baker [240]. They could assign a threshold electron energy at $\sim$185 keV to the displacement of zinc atoms in the lattice and 300 keV to tellurium atom displacement. This suggests a displacement energy of 7.35 eV for Zn atoms and 6.7 eV for Te.

In summary, the displacement energy values selected for calculations are: 5.6 eV for Cd atoms, 7.35 eV for Zn and 7.25 eV for Te atoms (averaging values for CdTe and ZnTe).
8.4. Displacement cross sections for CZT

The behaviors of PKA and displacement cross sections with the secondary electrons kinetic energy are shown in figure 8.2. This figure shows that, as expected from previous section, probability of atom displacements is non zero only for secondary electrons energies higher than about 185 keV for Zn, 235 keV for Cd and 323 keV for Te atoms. It means that for the studied sources, atom displacements will be expected for all atomic species. When the photon energy overcomes 333 keV threshold for the Zn cascade phenomenon begins to take place. This threshold energy is 412 keV for Cd and 552 keV for Te, as it is indicated by arrows in figure 8.2. It is observed that Cd atoms present the higher displacement cross section for electron kinetic energies higher than 298 keV. The cross section for Zn atoms shows the most gentle energy dependence, being the lowest for electrons with kinetic energies higher than 737 keV.

The McKinley-Feshbach approximation for the displacement cross section should gives difference higher than 1% (but still acceptable for our purposes) for Cd ($Z=48$) and Te ($Z=52$) atoms.

8.5. Determination and analysis of dpa distributions

Applying the MCCM procedure, the number of displacement per atom is calculated. First the total dpa value in each one of the 24×24 pixels of the CZT detector is calculated in order to evaluate the dpa spatial distribution in the pixelated matrix detector. Figure 8.3 shows the results for both studied gamma sources. The dpa damage accumulates quite homogeneously in all the pixels, even more for lower energy sources. The dpa values in the border pixels are about 93% of the value calculated in the central pixels for 511 keV incident photons and about 82% for irradiation with a $^{22}$Na source. It is also observed that photons from $^{22}$Na source produce displacement damage in one order of magnitude higher than 511 keV photons.

The total dpa in CZT matrix detector is now taken as the averaged sum over all pixels, obtaining $1.26\cdot10^{-28}$ and $1.72\cdot10^{-27}$ dpa per incident photon from 511 keV and $^{22}$Na sources respectively. The dpa produced by 511 keV photons is only about 7% of dpa induced by $^{22}$Na source. The contribution from each atom to the total dpa induced by each source is also calculated. In corresponding with their higher displacement cross section, the Cd atoms show higher number of atom displacement defects for both sources.
Displacement damage by gamma rays in a CZT matrix detector

Figure 8.2.: PKA (dashed lines) and displacement (solid lines) cross sections for all atoms in CZT. Arrows indicate the energy value where the cascade processes start.

Figure 8.3.: Mapping distribution of total dpa induced in 24×24 CZT pixel matrix detector by both studied sources.

Cd-dpa contribution is about 78% of the total dpa induced by 511 keV photons and about 65% of the case of $^{22}$Na source. Zn atoms are the least displaced, with only $\sim$10% and 5% contribution for 511 keV and $^{22}$Na gamma sources respectively. The corresponding contributions from Te atoms are then about 12% and 30%.

The displacements per atom distributions with the detector depth are also calculated. For this calculation the central pixel of the matrix detector is selected. Behaviors of in-depth dpa induced by both used gamma sources are presented in figure 8.4(a). Higher
dpa radiation damage in the whole volume of the detector is observed with the $^{22}$Na source. It is observed that atom displacements increase as radiation penetrates the detector pixel in both cases, excluding the first and last voxels.

In the proximity of the CZT-electrode interfaces a dpa radiation damage increment is obtained. This phenomenon is a consequence of the Au electrodes presence, with high atomic number ($Z=79$) and then high probability of electron production and backscattering processes. The electrons produced in the electrodes, and those produced in the CZT in the direction of the electrodes that are scattered back to the detector, contribute to the displacements formation processes inside the CZT in the electrodes vicinity.

The mean energy, calculated through (4.23), of the electrons produced in the top electrode is about 271 keV when irradiating with 511 keV photons. Electrons with this energy can penetrate up to 0.2 mm in CZT. This means that the electrons produced in the top electrode can contribute to dpa in the first voxel (0.2 mm length) of the CZT region. The mean electron energy is $\sim$422 keV when the $^{22}$Na source is used. In this case electron range is about 0.4 mm. Thus electrons coming from the top electrode can reach the second voxel inside the CZT, contributing then to dpa formation in the first two voxels. This fact is observed in the insets of figure 8.4(a), dpa is higher in the first voxel for the case of 511 keV photon source and in the first and second voxels in the case

![Figure 8.4:](image)

**Figure 8.4:** (a) Dpa in-depth profiles in CZT detector pixel produced by 511 keV and $^{22}$Na photon sources; insets show a magnification of these profiles for the first four voxels. (b) the same in (a) but removing the electrodes.
of $^{22}$Na source. In the CZT region near to the bottom electrode a drastic increase of the dpa value is also obtained. This is also related to the previous analysis, evolving the electrons produced in the electrode that enter in the CZT. In addition, the secondary electrons that leave the CZT in the electrodes direction can be backscattered again in the CZT material, contributing to further atom displacements formation.

In order to confirm all this, similar simulations removing both electrodes were performed. In this case the behavior of the dpa profiles are similar to those obtained above, increasing for deeper positions inside the CZT, as it is shown in figure 8.4(b). But the dpa values are lower for the first and last voxels, as expected in the absence of the Au electrodes. The results show that when irradiating with 511 keV photons the presence of the Au electrodes makes that the dpa values increase in 10% and 38% in the first and last voxel respectively. When using the $^{22}$Na source that increment is even higher, being in about 25% and 91% for the same voxels.

Finalizing this study, a comparison with similar calculations with the same detector geometry, but based on other usually employed materials, is carried out with the $^{22}$Na source. The semiconductor materials considered are crystalline silicon (c-Si) and gallium arsenide (GaAs). The displacement energies used for dpa evaluation are 15 eV for Si [82] and 10 eV and 15.5 eV for Ga and As atoms respectively in GaAs [242]. It is observed in figure 8.5 that the dpa values in the CZT detector are higher than in c-Si and GaAs in

![Figure 8.5: In-depth displacements per atom profiles in different detectors provoked by $^{22}$Na gamma source.](image)
the whole detector depth. The lower dpa values are obtained for the c-Si detector. This indicates that CZT gathered less dpa damage from gamma radiation than the other two studied materials. Quantitatively the dpa formation in CZT is 4.9 times higher than in GaAs and 7.9 times higher than in c-Si.

### 8.6. Dpa to energy deposition ratio

The in-depth energy deposition profiles in the studied CZT detector is also calculated through MCNPX for both gamma sources, as shown in figure 8.6. Photons from both sources deposit higher energy as the radiation goes deeper in the sample, remarking the values in the first and last voxels due to the presence of the electrodes. Irradiating with 511 keV photons a higher increase with depth is observed than with the $^{22}\text{Na}$ source. Photons and electrons produced by $^{22}\text{Na}$ source are more energetic than those due to 511 keV source and hence deposit more energy when they enter CZT region. But they also travel higher distances, about the double in CZT material. Then, more photons and electrons produced by 511 keV source will deposit its energy inside the CZT region.

The dpa to energy deposition ratio is calculated taken the total values for dpa and energy deposition inside the CZT detector pixels. Table 8.1 presents these results for both analyzed gamma sources. A similar calculation is performed for c-Si and GaAs.

![Energy deposition by different gamma sources in CZT.](image)
Table 8.1.: Dpa to energy deposition ratios in CZT for both studied gamma sources. Corresponding ratios for c-Si and GaAs by $^{22}$Na source are also included for comparison purposes.

<table>
<thead>
<tr>
<th>$\gamma$ source</th>
<th>$\eta \pm \Delta \eta \ (10^{-22}\ dpa/\text{MeV})$</th>
<th>CZT</th>
<th>c-Si</th>
<th>GaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>511 keV</td>
<td>0.472 $\pm$ 0.028</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$^{22}$Na</td>
<td>4.614 $\pm$ 0.213</td>
<td>2.611 $\pm$ 0.151</td>
<td>1.299 $\pm$ 0.071</td>
<td></td>
</tr>
</tbody>
</table>

considering the $^{22}$Na source for comparison purposes and the results are also included in Table 8.1. The dpa production per MeV of energy deposition by 511 keV photons is almost one order of magnitude (9.8 times) lower than the corresponding by $^{22}$Na source. Comparing with other semiconductors, CZT is more liable to dpa production per energy deposition unit than c-Si and GaAs. The dpa to energy deposition ratio induced by $^{22}$Na source in CZT is 1.8 times higher than in c-Si and 3.6 times higher than in GaAs.

8.7. Chapter conclusions

In this chapter the gamma radiation damage in terms of dpa induced by 511 keV and $^{22}$Na point sources in cadmium zinc telluride detectors was analyzed.

The dpa damage accumulates quite homogeneously in all the detector pixels, being one order of magnitude higher for a $^{22}$Na irradiation source than by 511 keV incident photons. The Cd atoms present the highest contribution to the total number of atom displacement defects for both sources, being the Zn atoms the least displaced.

The in-depth dpa distributions were calculated inside the matrix detector. It was observed that atom displacements induced by both studied sources increase as radiation penetrates deeper into the detector. Near the Au electrodes the dpa radiation damage rises drastically inside CZT matrix, via the release of electrons in the CZT-electrodes region and their backscattering in the electrodes.

The dpa to energy deposition ratio inside the CZT detector was calculated, being about 9.8 times higher for the $^{22}$Na source than for 511 keV incident photons. That is, the CZT material is more liable to dpa formation for more energetic irradiation gamma sources.
A comparison of CZT with alternative semiconductors crystalline silicon and gallium arsenide was performed using the $^{22}$Na source. It was observed that the dpa damage gathered by the CZT detector is about 8 times higher than by c-Si and about 5 times higher than by GaAs in the whole detector volume. This indicates that CZT material is more sensitive to gamma radiation damage in terms of dpa than the c-Si and GaAs materials. Also, the CZT has a higher dpa to energy deposition ratio than c-Si and GaAs. Displacements per MeV of energy deposition by photons from a $^{22}$Na source in c-Si and GaAs are respectively 56% and 28% lower than in CZT based detector.
Summary

“It is through science that we prove,
but through intuition that we discover.”
— Jules Henri Poincaré (1854–1912)

The work presented in this thesis aims to establish a method to evaluate the gamma and electron radiation damage in terms of Atom Displacements (AD). The proposed Monte Carlo assisted Classical Method (MCCM) relates the Oen-Holmes and Cahn established theories [3,4] about atom displacements to the electron and positron fluence distributions calculated from the Monte Carlo simulation. The proposal mainly consists in replacing the analytical distributions of particles produced in gamma and electron interactions with material by those obtained through the Monte Carlo simulation of radiation transport in matter.

Full comparisons between MCCM and previous theoretical estimations were presented and discussed. The main difference was found to be related to the secondary particle spectra considered for calculations. An overestimation in about 10-90% for the gamma irradiation induced dpa cross section from the previous evaluations was observed on regard to the MCCM results. On the contrary, the dpa cross section values produced by irradiation with electrons are underestimated in about 5-50% by the “classical” approximations when compared to the MCCM calculations. When thin samples are irradiated with electrons, the previous established methodologies lead again to an overestimation in about 20-70% related to the more precise results obtained through the MCCM.

The thesis presented in detail the calculation of the displacements per atom distributions in some technologically relevant materials and devices, like the YBa$_2$Cu$_3$O$_7$ superconductor ceramic and radiation detectors for medical applications based on lutetium-yttrium oxyorthosilicate and lutetium-yttrium orthoaluminate scintillators and cadmium zinc telluride semiconductor.
In the former studies in YBCO, the oxygen displacements in chain and plane crystalline sites at low gamma irradiation energies were analyzed, resulting that the contribution from the $O_c$ atoms dominates the total calculated dpa values. The results for higher incident gamma energies showed that the dpa damage increases drastically with depth, even more than one order of magnitude in the sample thickness for $E_\gamma \geq 3$ MeV. The positron treatment for dpa calculations in gamma radiation damage studies was found to be important. The positron contribution is small for low incident energy and increases with this last one. When positrons were considered in the calculation, the total dpa increases with the gamma irradiation energy. The results considering both electrons and positrons gave lower dpa values than the case of considering positrons as electrons. When positrons were neglected the dpa values decreased on regard to considering both electrons and positrons. In contrast with the case of gamma irradiation, the behavior of electron irradiation induced dpa is quite different. At higher energies dpa profiles become smoother and monotonously decreasing. This indicates that dpa values distribute more homogeneous in depth at higher electron irradiation energies. The dpa values produced by electron irradiation were about three order of magnitude higher than the dpa values induced by the gamma irradiation. This way the electron irradiation was more effective in provoking dpa damage inside the material than the gamma irradiation.

Later studies on the radiation damage in dpa terms induced by different gamma sources irradiation in LYSO and LuYAP crystals were presented. The dpa damage in LYSO crystals was higher than in LuYAP crystals, but the difference between dpa produced in LYSO and LuYAP decreased when more energetic sources were used. Interchanging the positions of LYSO and LuYAP crystals block inside the phoswich detector, the results allowed to conclude that the LuYAP crystals get a lower dpa exposure than the LYSO crystals. The total dpa damage in the whole detector block (LYSO + LuYAP) for the LuYAP-LYSO configuration was lower than for the LYSO-LuYAP case for all the studied sources.

Last, the gamma irradiation induced dpa damage in cadmium zinc telluride detectors was analyzed. The in-depth dpa distributions increase as radiation penetrates deeper into the detector. Near the Au electrodes the dpa radiation damage rises drastically inside CZT matrix, via the release of electrons in the CZT-electrodes region and their backscattering in the electrodes. It was observed that the dpa damage accumulated in the CZT detector is higher than the corresponding in the alternative c-Si and GaAs semiconductor based detectors.
On the other hand, based on the good correlation found between the dpa and energy deposition profiles for each incident energy in all the studied materials, it was possible to evaluate the dpa to energy deposition ratio. It was found in all the cases that the gamma and electron radiation energy deposition process supports better the atom displacement production at higher incident energies. In the case of YBCO HTS, the irradiating with electrons gave a dpa to energy deposition ratio that doubles the corresponding in the case of gamma irradiation for low irradiation energies, and was about 17 times higher for 10 MeV irradiation energy.

All the results within this thesis support the fact that applying the Monte Carlo simulation to obtain the secondary electron fluence distributions allows to take into account more realistic distributions in any point of the solid matrix. On the other hand, direct theoretical calculations can not evaluate the dpa volume distributions inside the material and do not consider the complex radiation transport phenomena and interactions. Therefore, the complex behavior of the gamma and electron interaction processes with matter can not be neglected at all for dpa calculations. MCCM methodology supports the introduction of a more reliable treatment for gamma and secondary electron/positron transport as demonstrated here with Monte Carlo based simulations. MCCM also allows to evaluate and study the dpa volume distributions inside the target material.
Samenvatting

“Het is door de wetenschap dat we bewijzen, maar door intuïtie die we ontdekken.”
— Jules Henri Poincaré (1854–1912)

In dit werk wordt voor het eerst een methode ontwikkeld om stralingsschade aangericht in kristallijne materialen geïnduceerd door hoogenergetische fotonen (gammastralen) en elektronen op basis van Monte Carlo methoden in detail te evalueren aan de hand van atoomverplaatsingsprofielen (displacement-per-atom of dpa profielen). In de voorgestelde Monte Carlo assisted Classical Method (MCCM) wordt de theorie van Oen-Holmes en Cahn aangewend om atoomverplaatsingen onder verschillende gamma en elektronen fluenties op stochastische wijze en met minder benaderingen te voorspellen. Met de voorgestelde techniek worden de analytische berekenbare gemiddelde verdelingen van secundaire deeltjes geproduceerd in materialen via de interactie van gammastralen en elektronen vervangen door een Monte Carlo berekening van microscopisch stralingstransport in materialen.

Een gedetailleerde vergelijking wordt gemaakt tussen MCCM en de voornoemende theoretische modellen. De conclusies hieruit zijn dat de analytische berekeningen de dpa werkzame doorsnede te wijten aan gammastraling overschat ten opzichte van MCCM, terwijl de dpa werkzame doorsneden te wijten aan elektronen bestraling de MCCM resultaten onderschat voor dikke proefstalen. In het geval van bestraling van dunne proefstalen met elektronen zullen de analytische methoden opnieuw de resultaten van MCCM overschatten. Het belangrijkste verschil tussen beide resultaten wordt toegewezen aan de keuze en de modelering van de spectra van secundaire deeltjes die verder in de berekeningen van atoom verplaatsingen worden aangewend.

Dit werk bevat een gedetailleerde studie van de atoomverplaatsingsprofielen geïnduceerd door straling in een aantal technologisch relevante materialen en stralingsde-
tectoren, zoals onder meer de YBCO keramische supergeleider en stralingsdetectoren voor medische toepassingen gebaseerd op scintillerend lutetium-yttrium orthosilicaat en lutetium-yttrium orthoaluminaat en de halfgeleider cadmium-zink-telluride. In het geval van de YBCO supergeleider werden de verplaatsingen van zuurstofatomen aanwezig in ketens \( O_c \) en in kristalvlakken \( O_p \) van de kristalstructuur apart onderzocht in het geval van bestraling met relatief laagenergetische gamma’s, met als resultaat dat de \( O_c \) atomen het totaal aantal atoomverplaatsingen domineert. Wanneer het staal bestraald wordt met hoogenergetische gammastralen \( E_\gamma \geq 3 \) MeV zal het aantal atoomverplaatsingen drastisch toenemen met verschillende grootte ordes naarmate men dieper in het materiaal kijkt. Hierbij is de behandeling van positron productie van toenemend belang bij toenemende energie van de invallende gammastraling. Het in rekening brengen van elektron-positron paar productie zal de totale hoeveelheid dpa doen toenemen. Wanneer men positronen op dezelfde manier behandelt als elektronen zal men echter het totale aantal dpa overschatten ten opzichte van de consistente behandeling van elektronen en positronen. Wanneer de productie van positronen wordt genegeerd onderschat men drastisch de hoeveelheid dpa, vooral bij hoge gamma energie.

In vergelijking met gamma bestraling zijn de geïnduceerde dpa profielen te wijten aan elektronen bestraling sterk verschillend. Bij hoge elektronen energie worden de dpa diepteprofielen vlakker en monotoon dalend hetgeen wijst op een meer homogene dpa verdeling onder invloed van hoogenergetische elektronen. De dpa waarden te wijten aan bestraling met elektronen is tot drie grootte ordes hoger dan de waarden verkregen bij gamma bestraling bij vergelijkbare energie, hetgeen impliceert dat stralingsschade drastischer is bij bestraling met elektronen dan bij bestraling met fotonen.

Verder worden in deze thesis de dpa profielen in LYSO en LuYAP kristallen onderzocht voor gammastralen afkomstig van verschillende stralingsbronnen. De stralingsschade in LYSO werd groter bevonden dan die in LuYAP, maar het verschil tussen beide wordt kleiner wanneer de energie van de straling toeneemt. Wanneer LYSO en LuYAP kristallen gecombineerd worden in een gamma detector voor medische PET diagnostiek zal het LYSO kristal dus meer stralingsschade oplopen, voornamelijk omwille van de geometrische configuratie waarbij het LuYAP kristal achter het LYSO kristal geplaatst wordt.

Tenslotte wordt de stralingsschade geïnduceerd door gammastraling aan de hand van dpa profielen onderzocht in detectoren gebaseerd op cadmium-zink-telluride (CZT). De dpa profielen als functie van de diepte in het staal groeien naarmate de straling dieper in het materiaal penetreert. Nabij de gouden contactelektroden in deze detectoren neemt de stralingsschade sterk toe door de toename van secundaire elektronen productie in
Au en door de terugstrooiing van elektronen in de elektrodes. De totale dpa schade geaccumuleerd in de CZT detector is groter dan die geïnduceerd door eenzelfde gamma fluentie in kristallijn silicium en galliumarsenide.

Tenslotte kan, door het vinden van een lineair verband tussen de totale dpa en de hoeveelheid afgestane energie van de straling in het materiaal, de hoeveelheid dpa per afgestane hoeveelheid energie worden bepaald als functie van de oorspronkelijke energie van de invallende straling. Hieruit concluderen we dat in alle bestudeerde gevallen zowel gamma als elektron irradiatie meer schade aanricht per afgestane hoeveelheid energie wanneer de oorspronkelijke energie het hoogst is. In het geval van de YBCO supergeleider is de dpa per gedeponeerde energie verhouding dubbel zo groot bij elektronen bestraling dan bij gamma bestraling bij lage energie en tot 17 keer groter wanneer de invallende stralingsenergie wordt opgedreven tot 10 MeV.

Alle resultaten uit deze thesis ondersteunen de hypothese dat het toepassen van een gedetailleerde Monte Carlo simulatie ter bepaling van de fluentie van secundaire elektronen en positronen te wijten aan bestraling van materialen een meer realistisch beeld geeft over de werkelijk aangebrachte stralingsschade. In tegenstelling hiermee zullen analytische methoden nooit de diepte profielen van de kans op atomaire verplaatsingen kunnen voorspellen en kunnen ze ook het gedetailleerde stralingstransport binnen materialen moeilijk bepalen. Daarom is MCCM, door het gedetailleerde modelleren van het stralingstransport en de meer correcte berekening van de aard en de hoeveelheid secundaire deeltjes, de aangewezen techniek om in detail de stralingsschade aangericht door irradiatie met elektronen en gamma stralen de bestuderen.
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List of figures

2.1. Formation of atom displacements when an incident particle impacts an atom from the atomic structure. .................................................. 8

2.2. Values for the ratio of the scattering to Rutherford-Darwin cross section. ................................................................. 14

4.1. The material volume could be subdivided in voxels for the Monte Carlo simulation process. .................................................. 32

4.2. Flowchart for atom displacements calculation through the MCCM procedure. ...................................................... 33

4.3. Main interface of the MCCM GUI tool. ........................... 37

5.1. Normalized effective electron energy fluence distributions for three incident gamma energies. .................................................. 41

5.2. Dpa cross sections calculated by Oen and Holmes [3] and MCCM in Cu for two values of the displacement energy. ........................ 44

5.3. Dpa cross sections in Si estimated by Cahn [4] and calculated by MCCM for two values of the displacement energy. ........................ 44

5.4. Dpa cross sections in Si according to Kwon and Motta [104] and MCCM for two values of the displacement energy. ........................ 44

5.5. Dpa cross sections in Fe by Fukuya-Kimura [54], Kwon-Motta [104], Baumann [101], Alexander [146] and MCCM. ........................ 44

5.6. Number of displacements per electron calculated by Oen and Holmes [3] and MCCM in Cu for two values of \( T_d \). ........................ 46

5.7. Number of displacements per electron in Si estimated by Cahn [4] and calculated by MCCM for two values of \( T_d \). ........................ 46

6.1. Crystalline lattice structure of YBCO superconductor. Both, planar and chain sites are indicated. ............................... 55

6.2. Displacement cross sections (a) as function of displacement energy for different incident energies and (b) as function of electron kinetic energy for both chain and planar sites. ............................... 57
6.3. Dpa in-depth distributions for oxygen atoms in the Cu-O chain and Cu-O$_2$ planar sites of YBCO superconductor. ................................. 58
6.4. Total oxygen dpa for each incident gamma energy in Cu-O chain and Cu-O$_2$ planar sites of YBCO superconductor. ................................. 58
6.5. In-depth energy deposition profiles for three gamma energies on YBCO. ................................. 60
6.6. Dpa dependence with energy deposition for three gamma ray energies. ................................. 60
6.7. Cutoff electron kinetic energy for different displacement energies for all atoms in YBCO. ................................. 62
6.8. Maximum kinetic energy of recoil atoms in YBCO. ................................. 62
6.9. Displacement cross sections for all atoms in YBCO. ................................. 64
6.10. In-depth dpa distributions for different incident gamma energies in YBCO. ................................. 65
6.11. In-depth displacement fluence profiles for different incident gamma energies in YBCO. ................................. 65
6.12. Atomic contributions to the total dpa in YBCO for different incident gamma energies. ................................. 66
6.13. O and Cu atom contributions to the total dpa in YBCO planar site for different $E_\gamma$. ................................. 66
6.14. In-depth energy deposition profiles in YBCO for different $E_\gamma$. ................................. 67
6.15. Dependence between dpa and energy deposition for different $E_\gamma$. ................................. 67
6.16. Displacements per atom to energy deposition ratios for different incident gamma energies. ................................. 67
6.17. (a) Displacement cross sections for electrons and positrons and (b) electron to positron displacement cross section ratios for all atoms in YBCO. ................................. 69
6.18. In-depth dpa distributions produced by electrons and positrons in YBCO for different gamma irradiation energies. ................................. 69
6.19. Contribution from electrons and positrons to the total dpa in YBCO at different gamma irradiation energies. ................................. 71
6.20. Total dpa in YBCO at different gamma irradiation energies considering different treatments for positrons. ................................. 71
6.21. Contributions from Cu-O$_2$ planes and Y and Ba atoms to total dpa in YBCO and from oxygen and copper atoms to dpa inside planar sites. ................................. 72
6.22. Displacements per atom to energy deposition ratios for different incident gamma energies. ................................. 73
6.23. In-depth dpa distributions in YBCO under different electron irradiation energies. ................................................................. 74
6.24. In-depth energy deposition profiles in YBCO for different electron irradiation energies. ................................................................. 74
6.25. Dpa induced by electrons and positrons in YBCO at different electron irradiation energies. ................................................................. 75
6.26. Displacements from Y and Ba atoms and from the Cu-O_2 planar site. . . 76
6.27. Contribution from oxygen and copper atoms to total in-plane dpa. . . . 76
6.28. Dpa to energy deposition ratios for different electron and gamma irradiation energies. ................................................................. 77

7.1. ClearPET® structure showing PMT detector cassette and crystals block. 83
7.2. Geometry, dimensions and properties of the model used for simulation. . 83
7.3. Displacement cross section for all atoms in LYSO and LuYAP crystals. . 86
7.4. Mapping distribution of total dpa induced in 8×8 LYSO crystals array by each one of the studied sources. ................................................................. 86
7.5. Total dpa produced by each gamma source in LYSO and LuYAP crystal matrices. ................................................................. 87
7.6. Total dpa produced by each gamma source in the whole detector block of CZT. ................................................................. 89
7.7. Individual contributions from each atom to the total dpa induced by different gamma sources. ................................................................. 89
7.8. Total dpa in-depth profiles induced in LYSO and LuYAP crystals by each studied source. ................................................................. 89
7.9. Dependence between dpa and energy deposition by different gamma sources in LYSO and LuYAP crystals. ................................................................. 91

8.1. Schematic representation of the simulated source-detector geometry. All the dimensions belong to a real small diameter PET. ................................................................. 95
8.2. PKA and displacement cross sections for all atoms in CZT. ...................... 97
8.3. Mapping distribution of total dpa induced in 24×24 CZT pixel matrix detector by both studied sources. ................................................................. 97
8.4. Dpa in-depth profiles in CZT detector pixel produced by 511 keV and^{22}Na photon sources. ................................................................. 98
8.5. In-depth displacements per atom profiles in different detectors provoked by $^{22}$Na gamma source. ................................................................. 99
8.6. Energy deposition by different gamma sources in CZT. .................. 100

List of tables

5.1. Electron-irradiation induced dpa values estimated in previous works and those calculated through MCCM. The relative difference between them is also showed. ................................................................. 47

6.1. Results from the linear fitting of the dpa vs. energy deposition dependences. The adjusted R-Square value for each fitting is also included. . . . . . . . . . . . . . . . . . . . . . . . 61

6.2. Values of $T_d$ and $n_k$ used to calculate $N_{dpa}$. The cutoff electron kinetic energies and the maximum kinetic energies of recoil atoms are also presented. 63

7.1. Dpa to energy deposition ratios in LYSO and LuYAP crystals for all studied gamma sources. Fitting adjusted R-Squares are also presented. . 91

8.1. Dpa to energy deposition ratios in CZT for both studied gamma sources. Corresponding ratios for c-Si and GaAs by $^{22}$Na source are also included for comparison purposes. ..................................................... 101
Glossary

$\Delta \eta$, standard deviation for the dpa to energy deposition ratio, 61
$\Omega$, particle scattering solid angle, 12
$\Phi$, radiation fluence, 11
$\Phi_0$, incident radiation fluence, 12
$\Phi_k$, fluence of electrons with energies in the range $[E_c^k, E_0]$, 33
$\Phi_\gamma$, gamma incident fluence, 40
$\Phi_C$, theoretical fluence of Compton electrons, 40
$\alpha$, fine-structure factor, 13
$\beta$, electron to light velocity ratio, 13
$\eta(E_0)$, displacements to energy deposition ratio, 35
$h$, crossed Plank’s constant, 13
$\nu(T)$, damage function, 17
$\sigma(E_0)$, radiation-atom total interaction cross section, 12
$\sigma^i(E_\gamma)$, gamma $i$-interaction cross section, 15
$\sigma_{PKA}$, PKA cross section, 30
$\sigma_c$, cross section for the production of Compton electrons, 40
$\sigma_{RD}$, Rutherford-Darwin electron scattering cross section, 13
$\sigma_R$, Rutherford charged particles scattering cross section, 12
$\sigma_{dpa}$, dpa cross section, 29
$\sigma_d$, displacements cross section, 31
$\theta$, electron scattering angle, 12
$\Phi_e(E)$, energy fluence distribution, 28
$\sigma(E, T)/dT$, interaction differential cross section, 11
AD, atom displacements, 27

c, light velocity, 13

\((-dE/dx)\), electron stopping power, 16
dpa, displacements per atom, 7

e, electron electric charge, 12

E, electron kinetic energy, 12

E_0, incident radiation kinetic energy, 12

E_c, electron cutoff energy, 10, 29

E_{dep}, energy deposition, 35

E_\gamma, gamma radiation energy, 15

E_{max}, maximum radiation kinetic energy, 11

f_k(E), probability distribution function that an electron possesses energy about E, 34

k, atomic species index, 28

M, atom rest mass, 10

m, electron rest mass, 10

mc^2, electron rest energy, 10

MCCM, Monte Carlo assisted Classical Method, 27

N_a, number of atoms per unit volume, 11

N_{AD}, number of atom displacements per unit volume, 28

N_{dpa}, number of displacements per atom, 29

N_e(E), energy distribution of secondary particles, 27

\pi(E_0), atom displacements produced over the range of an electron with energy E_0, 16

n_k, relative fraction of the k-atom in its crystalline sublattice, 28

N_T, total number of primaries per unit volume, 11

PKA, primary knock-on atom, 11
$Q$, atom displacements per length rate, 33

$r$, simulation estimated relative error, 23

$r_0$, electron classic radius, 30

$R$, ratio of the scattering cross section to Rutherford-Darwin one, 13

$R_C$, ratio of the Curr to Rutherford-Darwin cross section, 14

$R_{McF}$, ratio of the McKinley-Feshbach to Rutherford-Darwin cross section, 13

$S$, the total section of the material (or voxel) surrounding the volume $V$, 28

$\sigma_d^*$, normalized displacement cross section, 28

$T$, atom kinetic energy, 11

$T_c$, superconducting critical temperature, 56

$T_d$, atom threshold displacement energy, 9

$T_{\text{max}}$, maximum kinetic energy of the recoil atom, 30

$V$, volume of the sample, 27

$v$, electron velocity, 13

$X_0$, electron effective range, 16

$Z$, atomic number, 12
PhD related publications


131


Brief Curriculum Vitae
Academic Education

2004–2006 Master in Nuclear Physics, Instituto Superior de Tecnologías y Ciencias Aplicadas, Cuba.
Estudio del Daño Radiacional en materiales sólidos mediante la simulación de procesos físicos (maximum qualification)
Supervisors: Dr. Carlos M. Cruz, Dr. Antonio Leyva

1999–2004 Bachiller in Nuclear Physics, Instituto Superior de Tecnologías y Ciencias Aplicadas, Cuba.
Balance Energético Detallado y Procesos de Desplazamientos Atómicos inducidos por la Radiación Gamma en el YBCO (Golden Award with the maximum qualification)
Supervisor: Dr. Carlos M. Cruz

Professional Experience

Vocational

2011–present Aggregate researcher, Department of Physics, CEADEN, Havana City, Cuba.

2011–present Head of the Physics Department, CEADEN, Havana City, Cuba.

2007–2011 Junior researcher, Department of Physics, CEADEN, Havana City, Cuba.

2005–present Adjoint Instructor Professor, Department of General Physics and Mathematics, InSTEC, Havana City, Cuba.

2005–present Adjoint Instructor Professor, Department of Physics, Centro Universitario José Antonio Echeverría (CUJAE), Havana City, Cuba.

2004–2006 Research student, Department of Physics, CEADEN, Havana City, Cuba.
Scientific research work related with the Master thesis
Research by contract at CEADEN, Havana, Cuba

1 Project supported by the PNA / Agencia de Energía Nuclear y Tecnologías de Avanzada (AENTA).

12 Projects supported by the PRN / AENTA.

2 International Projects supported by the International Atomic Energy Agency (IAEA).
2009–2012 Technical Cooperation Project CUB7007
2005–2008 ARCAL LXXX Project RLA/7/011

2 Projects supported by the PNNMMA / Higher Education Ministry.

Conferences and Workshops: 44 (last 5 years listed)

22 International’s & 22 National’s

2014 XIII Simposio y XI Congreso de la Sociedad Cubana de Física, Havana, Cuba.
March 17–21. One Oral and Six Poster Presentations

February 5–8. Six Poster and Four Oral Presentations
Conference and Workshop Presentations: 72
49 International’s & 23 National’s

Publications: 32
+ 43 in Proceedings

Honors, Awards & Fellowships

Awards
2012 Award of the Cuban Academy of Science, for the Annual Scientific – Technical Outcome.
2008 AENTA Award for Young Researcher, for the significant contribution to scientific development.

Fellowships
2012 IAEA Fellowship, Irradiation by PIXE of particulate matter aerosol samples, Ruder Bošković Institute (RBI), Zagreb, Croatia, Ref.No. CUB11029. April 15 – May 15.
2010 ICTP Fellowship, to assist to the Advanced Workshop on Multi-scale for Characterization and Basic Understanding of Radiation Damage Mechanics in Materials, International Centre for Theoretical Physics (ICTP), Trieste, Italy, April 12–23.


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**Visits to Foreign Institutions**


2012 **Ruder Bošković Institute (RBI)**, Zagreb, Croatia, 1 month, April – May.

2010 **International Centre for Theoretical Physics (ICTP)**, Trieste, Italy, 2 weeks, April.

2008 **International Centre for Theoretical Physics (ICTP)**, Trieste, Italy, 2 weeks, November.


2007 **Centro de Capacitación en Calidad**, Mexico D.F., Mexico, 1 week, May.

2005 **Comisión Nacional de Energía Atómica (CNEA)**, Buenos Aires, Argentina, 1 week, December.

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**Professional Services**

**Conference/Workshop organizer:**

2009-2011-2013 **Member of the Organizing Committee of the WONP-NURT**.

2012 **Member of the Organizing Committee**, Latinoamerican Workshop on High Energy Physics: Particles and Strings, Supported by the ICTP and CERN. Havana City, Cuba. July 16–21.

**Proceedings editing:**

2009-2011-2013 **Proceedings of the WONP-NURT**.

**Reviewer/Referee:**

2010-2012 **Reviewer**, AENTA Annual Award nomination.


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**Memberships**

2012–present **American J. of Physical Chemistry, Science Publishing Group, USA**, *Editorial board member*.

2011–2014 **Physics Cuban Society**, *Secretary of the Nuclear, Atomic and Molecular Section*.

2009 **Institute of Electrical and Electronics Engineers (IEEE)**, *Student Member*.

2005–present **Physics Cuban Society**, *Member*.

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**Languages**

- **Spanish** Native language
- **English** Intermediate level
  
good reading, good writing, good understanding, average speaking

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**References upon request**