UNIVERSIDAD DE CÓRDOBA

Facultad de Ciencias

Grado de Física

Trabajo Fin de Grado

Luminescent response study of ionic crystals used in dosimetry

Código del TFG: FS24-008-FSC

Tipo de TFG: Trabajo de iniciación a la investigación

Autor: Marta de la Rosa Núñez



Agradecimientos

Incluir los agradecimientos, si procede. $\,$

Índice general

Índice general	2
Índice de figuras	3
ndice de tablas	
Resumen. Palabras clave	5
Abstract. Keywords	6
1. Introduction	7
2. Objectives	8
3.1. About LiF:Mg,Ti	9 9 9 11
4. Simulations	12
Conclusiones	
Conclusions	
Bibliografía	
Anexo: Ejemplo para introducir código Matlab	
Anexo: Ejemplo para introducir código ISE	

Índice de figuras

3.1.	Fermi-Dirac distribution for a semicoductor that is irradiated	10
3.2.	Schematic representation of the theoretical model	11

Índice de tablas

Resumen

Escriba aquí un resumen de la memoria en castellano que contenga entre 100 y 300 palabras. Las palabras clave serán entre 3 y 6.

Palabras clave: palabra clave 1; palabra clave 2; palabra clave 3; palabra clave 4

Abstract

Insert here the abstract of the report with an extension between 100 and 300 words.

Keywords: keyword1; keyword2; keyword3; keyword4

Introduction

As a bystander, one may pass life without thinking of the things that surrounds us. One may have had the misfortune of entering on an MRI, or the responsability to carry a dosimeter in a nuclear plant, and stepped out the room as it is. Life can go on unquestioned, and one may step out of that PET scan without thinking of the source of that awful noise.

Luminescence-based methods for detecting ionizing radiation have played a central role in radiation research since the earliest discoveries of radiation, radioactivity and atomic structure. These techniques exploit the ability of specific materials to emit light when exposed to ionizing radiation. This emitted light intensity is proportional to the radiation dose, making it possible to measure and to quantify the exposure.

One of the most commonly used materials in this context is lithium fluoride doped with magnesium and titanium (LiF:Mg,Ti). This material exhibits thermoluminescence, a phenomenon where trapped electrons in the crystal lattice are released upon heating, emitting light in the process. The study of such materials is crucial for improving the accuracy and efficiency of radiation detection systems, and it will be the cornerstone of this work.

Objectives

Theoretical framework

3.1. ABOUT LIF:MG,TI

Lithium fluoride (LiF) is a crystalline material that has been widely used in radiation dosimetry due to its favorable properties. It first appeared as a thermoluminescent dosimetry material in the 1950's, and since then, it has been extensively studied in the field of radiation detection. The material is composed of lithium (Li) and fluor (F) atoms, forming a crystal lattice structure of a face-centered cubic (FCC) type. Without any impurities, LiF is a semiconductor, with a bandgap of approximately 14 eV, which makes it an excellent insulator at room temperature.

To enhance the properties for radiation detection, LiF is often doped with magnesium (Mg) and titanium (Ti) ions, and sold commercially as TLD-100 [2]. The doping process introduces defects in the crystal lattice, creating energy levels within the bandgap. These defects play a crucial role in trapping and releasing charge carriers, which are responsible for the thermoluminescent response of the material. This process is known as thermoluminescence (TL), where the trapped electrons are released upon heating, resulting in the emission of light. The intensity of this emitted light is proportional to the amount of radiation absorbed by the material, making it a valuable tool for dosimetry.

3.2. The mathematical model

To describe the thermoluminescent response of a semicoductor, we can use a mathematical model based on the trapping and releasing of charge carriers in the accesible energy levels of the material.

Let us first consider the case of an arbitrary semicoductor without impurities. The energy levels of the conduction band and the valence band are separated by a bandgap

 E_g , and can be obtained with Schrodinger's equation that is under the influence of a periodic potential:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = E \ \psi(\vec{r}), \tag{3.1}$$

The periodicity of the potential $V(\vec{r})$ for any lattice vector \vec{R} allows the Bloch's theorem to apply, and so it gives rise to the formation of a band structure, composed by the conduction band, which is typically fully occupied at absolute zero temperature, and the valence band, which is in turn typically empty -or rather, we can consider it filled with holes (h^+) , or "positively charged electrons". The bandgap E_g is then defined as the energy difference between the top of the valence band and the bottom of the conduction band, and for a perfect crystal, no energy states are allowed in that region. This can be clearly seen if we take into account the density of available states, D(E), which is a function of the Fermi-Dirac distribution f(E) for a certain temperature T. This function gives the occupancy of any energy level E, and can be expressed as:

$$f(E) = \frac{1}{e^{\frac{E - E_f}{k_B T}} + 1},\tag{3.2}$$

Where E_f is the Fermi Level, and k_B is the Boltzmann constant. If the system is in equilibrium, and we set the case of T = 0K, the occupancy function f(E) will be equal to 1 for all energy levels below the Fermi level, and 0 for all energy levels above it. This means that the occupancy function will be a step function, with a discontinuity at the Fermi level, and so we can see that there are no available states in the bandgap region.

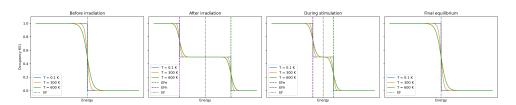


Figura 3.1: Fermi-Dirac distribution for a semicoductor that is irradiated.

The introduction of impurities or defects however, break the periodicity of the lattice, and create localized energy levels inside this "forbidden region". These levels can be thought of as traps for electrons if we are situated above the fermi level, and traps of holes if we are situated below. When this material is irradiated, electrons from the valence band can be excited to the conduction band, creating an electron-hole pair; and so changing the shape of the occupancy function. Once excited, both electrons and holes get "trapped" in these localized energy levels, and the excitation of these pairs into equilibrium will result in the emission of energy. In Figure 3.1 we can see a broad description of the perturbation of the system from its equilibrium state due to the irradiation, and the return of the system to equilibrium during either thermal stimulation or optical stimulation. If said relaxation processes are radiative, TL and OSL result.

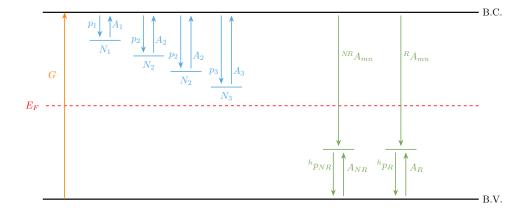


Figura 3.2: Schematic representation of the theoretical model.

And so, we can se a schematic representation of our theoretical model in Figure 3.2. Situating the energy in the Y axis, the focus is set in the energy gap of our material. Drawn in blue

3.3. The frequency factor

Simulations

Conclusiones

En este trabajo \dots

Conclusions

In this work ...

Bibliografía

- [1] Bellomo, N., Preziosi, L., Modelling and mathematical problems related to tumor evolution and its interaction with the immune system. *Mathematical and Computer Modelling*, **32**, pp. 413–452, 2000.
- [2] Y. S. Horowitz, L. Oster, and H. Datz, The thermoluminescence dose response and other characteristics of the high-temperature TL in LiF:Mg,Ti (TLD-100), *Radiation Protection Dosimetry*, vol. 124, no. 2, pp. 191–205, Jun. 2007, doi: 10.1093/rp-d/ncm241.

Anexo: Ejemplo para introducir código Matlab

```
%% 3-D Plots
  % Three-dimensional plots typically display a surface
  % defined by a function in two variables, z = f(x,y).
  %%
4
  % To evaluate z, first create a set of (x,y) points
  % over the domain of the function using meshgrid.
      [X,Y] = meshgrid(-2:.2:2);
      Z = X .* exp(-X.^2 - Y.^2);
  %%
9
  \% Then, create a surface plot.
10
      surf(X,Y,Z)
11
12
  % Both the surf function and its companion mesh display
  % surfaces in three dimensions. surf displays both the
  % connecting lines and the faces of the surface in color.
  % Mesh produces wireframe surfaces that color only the
16
  %lines connecting the defining points.
```

Anexo: Ejemplo para introducir código ISE

```
library IEEE;
                 use IEEE.STD_LOGIC_1164.ALL;
                use IEEE.STD_LOGIC_ARITH.ALL;
3
                use IEEE.STD_LOGIC_UNSIGNED.ALL;
4
   - Uncomment the following library declaration if
5
   -- instantiating any Xilinx primitive in this code.
   - library UNISIM;
   -- use UNISIM.VComponents.all;
9
  entity counter is
       Port ( CLOCK : in
                           STD_LOGIC;
       DIRECTION :
                      in
                           STD_LOGIC;
12
       COUNT_OUT :
                     out STD_LOGIC_VECTOR (3 downto 0));
13
  end counter;
14
  architecture Behavioral of counter is
16
   signal count_int : std_logic_vector(3 downto 0) := "0000";
17
  begin
  process (CLOCK)
  begin
20
       if CLOCK='1' and CLOCK'event then
21
           if DIRECTION='1' then
22
               count_int <= count_int + 1;</pre>
23
24
           else
               count_int <= count_int - 1;</pre>
25
           end if;
26
       end if;
27
  end process;
28
  COUNT_OUT <= count_int;
29
  end Behavioral;
```