Analysis of Electron Transport and Luminance Mechanisms in SrS Based Blue Emitting ACTFEL Devices

Praveen Sivakumar
University of Kentucky, pksu2003@hotmail.com

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ABSTRACT OF THESIS

The purpose of this thesis is to contribute to the understanding of SrS based ACTFEL devices. Better understanding of the processes in the host phosphor will give us the possibility to design more efficient blue emitting ACTFEL devices.

Towards this aim, a physical model, that describes the optoelectronic processes taking place in the phosphor, was developed and analytical equations were written. The analytical model was numerically simulated and the plots of flux flowing through the device and luminance output by the device were obtained. Experiments were performed to obtain the plots of current flowing through the device and luminance output by the device. These plots were then qualitatively compared and the results of comparisons are presented. The numerical simulations qualitatively verify the accuracy of the model.

The drive parameters were varied in order to study its effect on the VIL characteristics of the device. On varying the voltage applied to the device and its rise and fall times, a good insight was obtained into device behavior. Simulations were also performed to obtain responses to qualitatively match the experimentally obtained responses.

Various What-If scenarios have been studied by varying the device parameters. These studies have indicated the importance of these parameters in determining device performance.

KEYWORDS: ACTFEL, Electroluminescent Displays, Flat Panel Displays, Phosphors, SrS

PRAVEEN SIVAKUMAR
August 21, 2003
Analysis of Electron Transport and Luminance Mechanisms in SrS Based Blue Emitting ACTFEL Devices

By

Praveen Sivakumar

Dr. Vijay P. Singh
Director of Thesis

Dr. William T. Smith
Director of Graduate Thesis
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ANALYSIS OF ELECTRON TRANSPORT AND LUMINANCE IN SrS BASED BLUE EMITTING A.C. THIN FILM ELECTROLUMINESCENT DEVICES

THESIS

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in the College of Engineering at the University of Kentucky

By
Praveen Sivakumar
Lexington, Kentucky

Director: Dr. Vijay P. Singh
Professor and Chair
Department of Electrical and Computer Engineering
University of Kentucky
Lexington, Kentucky
2003
Dedicated to my
Dad, Mom and Sister
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Chapter 1
INTRODUCTION

1.1 Electroluminescence

Electroluminescence (EL) is the phenomenon by which light is generated by applying an electric field to a substance. Light is generated by impact excitation of a light-emitting center, called an activator, by high energy electrons whose energy is due to their acceleration in a high electric field.

1.2 History of Electroluminescence

Electroluminescence was accidentally discovered by Distriau in 1936 when he was working with ZnS compound. In 1967, Russ and Kennedy reported electroluminescence in ZnS:Mn phosphor sandwiched between insulators[1]. The phosphor layer was placed between two layers of insulator in these devices. However, these devices had a short lifetime. In 1969, Vlasenko and Popkov observed that thin film ZnS devices had much better characteristics than its powder counterparts[1]. In 1974, long life device were fabricated by Inoguchi and shortly after, Mito showed that these devices could be used for television imaging[1].

The first commercial thin-film EL products were introduced by Sharp in 1983. In the same year, Grid announced the first portable computer which used a 6-inch diagonal 320x240 pixel EL display panel. In mid 80’s Sharp, Finlux and Planar Systems introduced half-page, 9-inch-diagonal yellow-emitting ZnS:Mn thin-film EL displays on the market and also offered a variety of EL products. Now, ZnS:Mn thin-film EL displays are readily available in different sizes up to full sizes for workstations[1].
1.3 Display Technologies

Displays are the most common means of presenting information in today’s world. There are many different display technologies currently in use. The most common technologies in use today are Cathode Ray Tube (CRT) and Flat Panel Displays (FPD).

1.3.1 Cathode Ray Tube

CRT technology is used most widely in today’s world. The reasons for its widespread use are its long life, good resolution, brightness and contrast controls, and color capabilities. However, the drawbacks are that they are bulky devices, require high voltage for operation, consume too much power and emit harmful electromagnetic radiation during operation. Moreover, large display units are difficult to manufacture because of the size of the Cathode Ray Tube.

1.3.2 Flat Panel Displays

An alternative technology that has taken the world by storm in recent years is Flat Panel Display. LCDs are synonymous with FPD technologies. They, being solid state devices, are rugged, lightweight, and portable and consume less power for their operation. It is also possible to manufacture 12-20 inch full-color liquid crystal displays. They suffer from some serious shortcomings like limited viewing angle and loss of visibility under sunlight. However, in spite of these drawbacks, LCDs find applications in computer displays.

Another flat panel display technology that is gradually finding acceptance is Plasma Display. They produce higher luminance and contrast and modest resolution of 32 dots per inch [1]. These advantages make them most suitable for use in large information screens and high-definition television applications. However, they are very expensive to manufacture.

1.3.2.1 ACTFEL Technology

A.C. Thin Film Electroluminescent (ACTFEL) technology have gained universal acceptance in demanding display applications where excellent viewing characteristics are necessary. They possess the following advantages:

1. They have good contrast and can be used in applications where good contrast must be maintained in a very high ambient illumination environment.
2. They have high legibility because light is emitted from a sub-micron thick device and the pixel edges are sharp.
3. They are light weight devices and have wide viewing angle (>160°).
4. They have very fast response time (few microseconds) [2].

These advantages make electroluminescent (EL) displays an attractive choice for medical or industrial instruments, military equipment, and virtual reality systems, where compactness is vital.

Despite the numerous advantages of EL technology over other FPD technologies, commercial full-color displays are not available yet, due to the absence of an efficient blue emitting phosphor. In order to produce a multi-color thin-film EL display, efficient red, green and blue phosphors need to be produced. Red and green colors can be filtered out from yellow emitting ZnS:Mn. However, highly efficient blue emitting thin-film EL displays still need to be produced. An understanding of the processes behind the light emission from the blue devices will serve to improve the luminous efficiency of the device.

1.4 Motivation

The purpose of this thesis is to contribute to the understanding of SrS based ACTFEL devices. Better understanding of the processes in the host phosphor will give us the possibility to design more efficient blue emitting ACTFEL devices.

Towards this aim, a physical model, that describes the optoelectronic processes taking place in the phosphor, was developed and analytical equations were written[2]. The analytical model was numerically simulated and the plots of flux flowing through the device and luminance output by the device were obtained. Experiments were performed to obtain the plots of current flowing through the device and luminance output by the device. These plots were then qualitatively compared and the results of comparisons are presented.
Chapter 2

THEORY

A physical model was developed to describe the optoelectronic processes in SrS:Cu ACTFEL devices. The structure of the ACTFEL device is presented in Section 2.1. The mechanism of electroluminescence is explained in Section 2.2. The model developed to describe electron transport and luminance mechanisms in these devices is described in Section 2.3.
2.1 ACTFEL Device Structure

The schematic of an ACTFEL device is shown in Figure 2.1.

![Figure 2.1: Schematic of an ACTFEL Device](image)

The base of the device is made up of thick glass, which gives mechanical support to the device. A film of Indium Tin Oxide (ITO), a transparent conductor, is coated on top of the glass substrate; it serves as one of the metal electrodes. During actual device operation, a high electric field is present across the device. Hence, any imperfection in the thin-film phosphor might produce a short circuit and cause the device to burn out, if the phosphor layer was directly connected to the electrode. To prevent the device from burning out, a thin film of an insulating layer is deposited on the ITO layer. This thin film insulator serves as a current limiting insulator. The active phosphor layer is deposited on top of the insulator. The second insulating layer is then deposited on the phosphor active layer. The two dielectric layers determine the threshold voltage, breakdown voltage, and the luminous efficiency of the device. A layer of aluminum is deposited on the insulating film and functions as the other metal electrode. The Aluminum back layer electrode also serves as a reflective layer to increase the luminous efficiency of the device. Hence, the light incident on aluminum from the phosphor is reflected back and the luminance produced from the device is collected from the glass side of the device.
2.2 Mechanism of EL Production in ACTFEL Devices

An overview of the EL emission process in SrS:Cu phosphor ACTFEL device is described below:

1. A voltage applied to the two electrodes of the ACTFEL device sets up an electric field across the phosphor. When the value of the applied electric field is above the threshold field required for tunneling, the electrons tunnel from the insulator-phosphor interface and accelerate towards the anode.

2. As the electrons accelerate in the high electric field (usually of the order of few MV/cm), their kinetic energy increases.

3. These high energy electrons, also known as “hot” electrons, impact the luminescent centers of the phosphor (For the device under consideration, the luminescent centers are Cu atoms). Upon impact, the electrons are excited from the lower to the higher energy level within the Cu atoms. When the electrons in the excited state of the phosphor make radiative transitions to the ground state, EL emission occurs. If the impacting electrons possess sufficient energy, they ionize the activators, leaving them positively charged. The released electrons can (i) end up in the conduction band of the phosphor and contribute to flux or (ii) get trapped in the host lattice. These trapped electrons form dipoles with the positively charged ionized activators in its vicinity. When the field in the phosphor is insufficient to maintain the dipoles, the dipole collapses and the electron returns to the higher energy level of the activator. Light is emitted when these electrons make radiative transitions to the ground state from the excited state.

4. The hot electrons, as well as the electrons impact ionized from the Copper atoms, travel through the phosphor layer and upon reaching the anodic phosphor/insulator interface, are trapped at the interface states. Due to the charge transferred from the cathodic interface to the anodic interface and ionization of activators in the phosphor, an internal electric field, that opposes the external applied electric field, is setup in the phosphor. Hence, the net electric field across the phosphor decreases and consequently, the flux of electrons tunneling from the cathodic interface also decreases.
5. When the voltage applied to the device falls to zero, the internal electric field in the phosphor causes the electrons to tunnel from the anodic interface. These electrons recombine with the ionized activators in the phosphor. Light is produced when these electrons make radiative transitions from the excited to the ground state.

### 2.3 Physical Model

The model, developed to describe the optoelectronic processes in SrS:Cu ACTFEL devices, is presented here. The electronic and luminance processes in the device are defined at various times $t_1$, $t_2$, $t_3$, $t_4$ and $t_5$ during the positive pulse at steady state (see Figure 2.2).

![Figure 2.2: Driving voltage waveform showing some significant times.](image)

At time $t = t_1$, the electric field in the phosphor is large enough to tunnel eject electrons from the insulator-phosphor interface at the cathodic end. The electrons that tunnel out of the cathodic interface are termed “hot electrons” because they possess high kinetic energy and this energy increases as they travel in an increasing electric field. These electrons impact the luminescent centers of the phosphor, termed activators. The activators are made up of Copper atoms. When the electrons impact the Copper atoms, electrons are excited from the lower energy level of the activator to the higher energy level. These electrons relax back to the state of lower energy and in the process emit light, whose wavelength is given by Planck’s equation,

$$\lambda \text{(in nm)} = \frac{1.24}{E_g \text{(in eV)}}.$$
The emission wavelength, thus calculated, is 450nm which corresponds to the wavelength of blue light.

Also, at time $t=t_1$, a fraction of the hot electrons possess enough energy to kick out electrons from the activator. This process is termed “impact ionization of activators by hot electrons”. The loss of electrons from the phosphor leaves the activators positively charged. Thus, impact ionization of activators in the phosphor creates a positive bulk space charge. Additionally, when the electrons leave the cathode, travel through the phosphor and get trapped at the anode, the anodic end develops negative charge while the cathodic end develops positive charge. Due to the two processes described above, an internal field is set up in the device across the phosphor ($E_{int}$) that opposes the direction of the applied field. This internal electric field is made up of two components: (i) constant electric field that is setup between the now positively charged cathode and the now negatively charged anode and (ii) steadily increasing electric field along the direction from the cathode to the anode due to the charges in the bulk phosphor and the negative charges at the anode. These two components add up to contribute to the internal electric field ($E_{int}$).

So, at time $t_1$, the impact ionization of Copper activators results in the release of an electron. This released electron can either end up in the conduction band of SrS ($Process \ P_2$) or be trapped by a “daughter “ bulk trap in the vicinity of the activator, thus creating a bulk dipole ($Process \ P_3$).

These dipoles are positively-charged-ionized-activator/negatively-charged-bulk trap pairs in close vicinity; the bulk trap is thought to be formed by the introduction of activator in the phosphor lattice and is, thus, intimately related to “its” activator. It is localized in the vicinity of its activator, and is termed the “daughter” trap [3]. A minimum electric field is required to maintain the dipole. This minimum electric field would be present at the leading edge of the driving voltage pulse when the dipoles are created. When the bulk phosphor field goes below this $E_{min}$ (which occurs when the driving voltage pulse is reduced), the field is no longer sufficient to maintain the dipole and hence the ionized activator recaptures the electron from its daughter trap. This results in the annihilation of the dipole and photon emission as the activator relaxes to the lower energy level.
At time $t_1$, due to the electric field in the phosphor, the electrons tunnel from the activators to the traps and the conduction band. This is termed as field assisted tunneling. The electrons in the bulk traps also tunnel to the conduction band of the phosphor.

The net phosphor field is reduced at the trailing edge beginning at $t = t_2$ (see Figure 2.2). Photon emission caused by the reduction in voltage will manifest as a luminance peak and is termed the BTE (Beginning of Trailing Edge) peak.

At time $t = t_2$, the BTE is experimentally observed. The electrons trapped in the “daughter” bulk trap transfer to the ionized activator in the vicinity (since the net electric field in the phosphor is no longer sufficient to maintain the dipole) causing the annihilation of the dipole resulting in the BTE luminance ($Process \ P5$).

Recombination between electrons in conduction band and holes in traps take place. The probability of this occurring is very low because the electrons in conduction band would rather fall to the positively charged activators than to the neutral traps.

At times $t = t_3$ and $t = t_4$, the electric field at the anodic end of the phosphor layer is negative because the internal electric field is now greater than the applied electric field. Electrons are therefore released from the shallow trap levels at the anodic interface states. These electrons can,

(i) Recombine with the ionized activators near the interface and cause MTE luminance ($Process \ P7$).

(ii) Accelerate in the negative electric field and impact excites Copper activators causing MTE luminance ($Process \ P8$).

Processes $P_1$ to $P_8$ define the various opto-electronic processes taking place in the bulk phosphor.
Chapter 3

ANALYSIS

This chapter is dedicated to a rigorous mathematical analysis of the physical model presented in the previous chapter. The chapter is divided into 4 sections:

1. Electric Field Distribution
2. Electron Tunneling from Interface States,
3. Charge Transfer and Luminance Processes in Phosphor Layer and
4. Electron Capture at Interface States.

Equations are presented in each section, for each of the processes described in the previous chapter, where the physical model for the optoelectronic processes was discussed.
3.1 Electric Field Distribution

The electric field in the device is determined by solving Poisson’s equation using appropriate boundary conditions.

Poisson’s equation is given by the expression,

\[ \Delta^2 \psi = -\frac{\rho}{\varepsilon} \]

.......................... (1) where, ‘\( \rho \)’ is the charge density; ‘\( \varepsilon \)’ is the permittivity of the medium and ‘\( \psi \)’ is the voltage.

\[ \text{Region A:} \]

There is no space charge in the insulator. Hence, the electric field is constant in this region.

\[ E_A(x) = C_1 \text{ Volts/cm} \]

.......................... (2)

Hence, the voltage in region A is,
\[
V_A(x) = C_1 x + C_2 \text{ Volts} \quad \text{.......................... (3)}
\]
Where, ‘\(C_1\)’ and ‘\(C_2\)’ are constants of integration and are solved from the boundary conditions.

**Region B:**

The phosphor section has a number of activators and mid-gap traps that are charged during device operation (For details, refer Section 2.3). It is assumed that the charge distribution on the planar area perpendicular to the ‘\(x\)’ direction is the same but the charge density could vary along the ‘\(x\)’ axis. Hence, the Poisson’s equation in region B is written as,

\[
dE/dx = \rho/\varepsilon \quad \text{.......................... (4)}
\]
Where, ‘\(E\)’ is the electric field and ‘\(\rho\)’ is the charge density.

The phosphor region is divided into ‘\(n\)’ sections and the charge density is approximately the same in each of the ‘\(n\)’ sections.

Thus for section ‘\(i\)’, \((W_1+(i-1)W_x<x<W_1+iW_x)\), the electric field is given by,

\[
E_B(i,x) = C_3(i) + (q/\varepsilon_Z)\rho(i)(x-(W_1+(i-1)W_x)) \text{ Volts/cm} \quad \text{.......................... (5)}
\]

The voltage in \(i^{th}\) section is given by,

\[
V_B(i,x) = C_3(i)[x-(W_1+(i-1)W_x)] + C_4(i) + (q/2\varepsilon_Z)\rho(i)[x-(W_1+(i-1)W_x)] \text{ Volts} \quad \text{.......................... (6)}
\]
where, ‘\(\rho(i)\)’ is the net positive charge density in section ‘\(i\)’, ‘\(\varepsilon_Z\)’ is the dielectric constant of SrS (9.4*8.854*10^{-14} Farads/cm) and ‘\(q\)’ is the electronic charge (-1.6*10^{-19} Coulombs).

**Region C:**

There is no space charge in the insulator, i.e. region C. Hence, the electric field is constant and is given by,

\[
E_C(x) = C_5 \text{ Volts/cm} \quad \text{.......................... (7)}
\]

The voltage in region C is

\[
V_C(x) = C_5[x-(W_1+W_Z)] + C_6 \text{ Volts} \quad \text{.......................... (8)}
\]

The constants ‘\(C_1\)’, ‘\(C_2\)’, ‘\(C_3\)’, ‘\(C_4\)’, ‘\(C_5\)’ and ‘\(C_6\)’ are solved from the boundary conditions.

Assume that the ITO is at ground potential and a positive voltage is applied to the Aluminum back electrode.

At \(x = 0\),

\[
V_A = 0 \quad \text{.......................... (9)}
\]
At \( x = W_1 \),
\begin{align*}
V_A &= V_B \quad \text{.................. (10)} \\
D_B - D_A &= q(n_{DC} + n_{SC} - n_{EQ}) \quad \text{.................. (11)}
\end{align*}

At \( x = W_1 + W_Z \),
\begin{align*}
V_B &= V_C \quad \text{.................. (12)} \\
D_C - D_B &= q(n_{DA} + n_{SA} - n_{EQ}) \quad \text{.................. (13)}
\end{align*}

At \( x = 2W_1 + W_Z \),
\begin{align*}
V_C &= V_A \quad \text{.................. (14)}
\end{align*}

where, ‘\( D_A \)’, ‘\( D_B \)’, ‘\( D_C \)’ are the dielectric displacements in regions ‘A’, ‘B’ and ‘C’, and
\begin{align*}
E_A &= D_A/\varepsilon_D, \quad E_B = D_B/\varepsilon_Z \quad \text{and} \quad E_C = D_C/\varepsilon_D \quad \text{.................. (15)}
\end{align*}

where, \( \varepsilon_D = 7.9*8.85*10^{-14} \text{ Farads/cm} \) is the dielectric constant of the insulator; ‘\( n_{SC} \)’ and ‘\( n_{DC} \)’ are the densities of electrons at the shallow and deep cathodic interface states, respectively; ‘\( n_{SA} \)’ and ‘\( n_{DA} \)’ are the densities of electrons at the shallow and deep anodic interface states, respectively; ‘\( V_A \)’ is the voltage applied to the anode.

Using the boundary conditions above, we can solve the constants:
\begin{align*}
C_2 &= 0 \quad \text{.................. (16)} \\
C_3(1) &= (\varepsilon_D C_1 - q(n_{SC} + n_{DC} - n_{EQ}))/\varepsilon_Z \text{ Volts/cm} \quad \text{.................. (17)} \\
C_4(1) &= C_1 W_1 \text{ Volts} \quad \text{.................. (18)} \\
C_3(i+1) &= C_3(i) + (q/\varepsilon_Z)\rho(i)W_x \text{ Volts/cm} \quad \text{.................. (19)} \\
C_4(i+1) &= C_3(i)W_x + C_4(i) + (q/2\varepsilon_Z)\rho(i)W_x^2 \text{ Volts} \quad \text{.................. (20)}
\end{align*}

where, ‘\( i \)’ varies from 1 to ‘\( n \)’; ‘\( n \)’ is the total number of sections of the phosphor.
\begin{align*}
C_5 &= (C_3(n)\varepsilon_Z + q \rho(n)W_x - q(n_{DA} + n_{SA} - n_{EQ}))/\varepsilon_D \text{ Volts/cm} \quad \text{.................. (21)} \\
C_6 &= C_3(n)W_x + C_4(n) + (q/2\varepsilon_Z)\rho(n)W_x^2 \text{ Volts} \quad \text{.................. (22)} \\
V_A &= C_5 W_1 + C_6 \text{ Volts} \quad \text{.................. (23)}
\end{align*}

### 3.2 Electron Tunneling from Interface States

When the driving voltage across the device is larger than the threshold voltage, the magnitude of the electric field that is set up in the phosphor is large enough to cause the
conduction band of the phosphor to bend. The barrier to the interface state electrons becomes thin and hence, the electrons tunnel out to the conduction band. This phenomenon is called Fowler-Nordheim tunneling. For the purpose of simulations, two states are assumed to be present at the phosphor/insulator interface and are appropriately called shallow and deep interface states.

Due to Fowler-Nordheim tunneling described above, the electron flux produced by tunneling from both the interface states is given by:

\[
F_e = f_{os} n_{sc} P_{sc}(F) + f_{od} n_{dc} P_{dc}(F) \text{ cm}^{-2} \text{s}^{-1}
\]  

……………….. (24)

where, ‘f<sub>os</sub>’ and ‘f<sub>od</sub>’ are the occupancy constants of the shallower and deeper interface states (taken as 1 for simulation); \(n_{sc}\) and \(n_{dc}\) are the density of electrons at the shallow and deep interface states; ‘\(P_{sc}(F)\)’ and ‘\(P_{dc}(F)\)’ are the probabilities of field ionization from the interface states,

\[
P_{sc} = a(m/m^*)^{1/8} (E_{sc})^{5/8} (F)^{1/4} e^{-b(m/m^*)^{1/2}} (E_{sc})^{3/2} (1/F)
\]  

……………….. (25)

\[
P_{dc} = a(m/m^*)^{1/8} (E_{dc})^{5/8} (F)^{1/4} e^{-b(m/m^*)^{1/2}} (E_{dc})^{3/2} (1/F)
\]  

……………….. (26)

where, ‘F’ is the electric field at the cathodic interface; ‘m’ and ‘m*’ are the mass and effective mass of an electron, respectively. ‘\(E_{sc}\)’ and ‘\(E_{dc}\)’ are the depths of the energy levels of the cathodic interface states measured from the conduction band. ‘a’ and ‘b’ are constants associated with the barrier.

Once the electrons tunnel out of the interface states, they are accelerated towards the anode to their saturation velocity because of the applied electric field [6].

### 3.3 Charge Transfer and Luminance Processes in the Phosphor Layer

The phosphor is doped with a large density of Copper activators given by ‘\(Na_0\)’ (\(cm^{-3}\)). It is also thought to contain traps whose density is given by ‘\(Nt_2\)’ (\(cm^{-3}\)) at energy level ‘\(E_1\)’ measured from the conduction band.

The various transfers of charge taking place between various levels in the phosphor are sketched in Fig 3.2.
Figure 3.2: Rate Diagram depicting the transfer of charge between the various energy levels, namely ‘$E_{AL}$’ (Lower Energy Level of the Activator), ‘$E_{AH}$’ (Higher Energy Level of the Activator), ‘$E_1$’ (Energy Level of the Bulk Trap) and ‘$E_C$’ (Energy Level of the Conduction Band of the Phosphor).

At this juncture, it is helpful to describe the various levels presented in Figure 3.1. ‘$E_{AL}$’ denotes the lower energy level of the activator; ‘$E_{AH}$’ denotes the higher energy level of the activator; ‘$E_1$’ denotes the energy level of the bulk trap and ‘$E_C$’ is the energy level of the conduction band of the phosphor. The energy difference between the lower energy level of the activator and the conduction band is 4.1 $eV$. The energy difference between the lower and higher energy levels of the activator (Cu) is 2.75 $eV$. The energy difference between the higher energy level of the activator and bulk trap is assumed to be 0.25 $eV$.

Rate Equation 1:

*The rate of electron transfer from lower energy level to the higher energy level of the activator through impact excitation is given by*

$$R_i = f_i(E)\alpha A$$

.......................... (27)
Where, ‘f’ is the flux of electrons (/cm$^2$s); ‘A’ is the area of the device (cm$^2$) (taken as unity); ‘E’ is the electric field (V/cm); ‘$f_1(E)$’ is the fraction of hot electrons flux with enough energy for impact excitation (= 0.05 for simulation); ‘α’ is the impact parameter is defined as

$$\alpha = u(x,t)\pi R^2$$

.......................... (28)

Where, ‘u(x,t)’ is the density of electrons at the lower energy level of the activator ($E_{AL}$) (/cm$^3$); ‘R’ is the radius for impact (cm) (= 100 Å for simulation).

**Rate Equation 2:**

*Charge transfer between Activator and Bulk Trap is given by:*

$$R_2 = R_{2A} + R_{2B}$$

.......................... (30)

Where ‘$R_{2A}$’ is the rate of the impact ionization from lower level activator states to bulk traps and is given by:

$$R_{2A} = f_2(E) f z(E) A \alpha$$

if $u(x,t) \leq p_T$

.......................... (31a)

$$R_{2A} = (p_T f_2(z(E))) A \pi R^2$$

if $u(x,t) > p_T$

.......................... (31b)

Where, ‘$f_2(E)$’ is the fraction of electron flux that has enough energy for impact ionization of electrons (= 0.01 for simulation); ‘$p_T$’ is the trap density (/cm$^3$); ‘$f_3(E)$’ is the fraction of electrons which are impact ionized to the trap level ‘$E_1$’ (= 0.6 for simulation); ‘R’ is the radius of a sphere surrounding the electron, within which the flux can cause impact ionization of electrons (radius of impact) (= 100 Å for simulation).

‘$R_{2B}$’ is the rate at which electrons undergo field assisted tunneling from lower level activator states to bulk traps and is given by:

$$R_{2B} = u(x,t) P_{EAL1}$$

if $u(x,t) \leq p_T$

.......................... (32a)

$$R_{2B} = p_T P_{EAL1}$$

if $u(x,t) > p_T$

.......................... (32b)

Where, ‘$P_{EAL1}$’ is the probability of field assisted tunneling from ‘$E_{AL}$’ to ‘$E_1$’.

$$P_{EAL1} = a(m^{1/8} / m^{*1/8})E_{L1}^{5/8} F_i^{1/4} \exp(-b(m/m^*)^{-1/2} E_{L1}^{3/2} / F_i)$$

.......................... (33)

Where, ‘$F_i$’ is the electric field in the $i^{th}$ section; ‘$E_{EAL1}$’ is the energy gap between ‘$E_{AL}$’ and ‘$E_1$’; ‘m’ and ‘$m^*$’ are the mass and effective mass of electron respectively; ‘a’ and ‘b’ are
constants associated with the barrier whose values are $9 \times 10^{10}$ and $1.49 \times 10^8$ respectively; ‘$p_T$’ is the density of empty bulk traps and is given by:

$$p_T = n_{t0} - n_{t2}$$  
............................ (34)

Where, ‘$n_{t0}$’ is the density of bulk traps in the phosphor layer; ‘$n_{t2}$’ is the electron density at trap level ‘$E_1$’.

**Rate Equation 4:**

Charge transfer from higher energy level to lower energy level is the luminance producing transition and its rate is given by

$$R_{q} = e(x,t)\gamma$$  
............................ (29)

Where, the parameter ‘$\gamma$’ is the relaxation rate of excited activators (sec) and is defined as the inverse of the relaxation time ($1/\tau_2$) ($\tau_2 = 0.05\mu s$); ‘$e(x,t)$’ is the density of electrons at the higher energy level of the activator ($E_{AH}$) (cm$^3$).

**Rate Equation 12:**

Similarly, electrons from the higher energy level of the activator can also end up in the bulk traps by either impact ionization or field assisted tunneling and this process is modeled by the rate equations ‘$R_{12A}$’ and ‘$R_{12B}$’.

$$R_{12} = R_{12A} + R_{12B}$$  
............................ (35)

$$R_{12A} = e(x,t)\gamma f_2^2(F) A\pi R^2$$  
if $e(x,t) \leq p_T$  
............................ (36a)

$$R_{12A} = p_T \gamma f_2^2(F) A\pi R^2$$  
if $e(x,t) > p_T$  
............................ (36b)

Where, ‘$f_2^2(F)$’ is the fraction of electron flux with enough energy for impact ionization of electrons in ‘$E_{AH}$’ (= 0.2 for simulation); ‘$p_T$’ is the trap density (cm$^3$); ‘$e(x,t)$’ is the electron concentration at the energy level ‘$E_{AH}$’.

The field assisted tunneling from the higher energy level of the activator ($R_{12B}$) is given by

$$R_{12B} = e(x,t)P_{EHE1}$$  
if $e(x,t) \leq p_T$  
............................ (37a)

$$R_{12B} = p_T P_{EHE1}$$  
if $e(x,t) > p_T$  
............................ (37b)
Where, ‘\(P_{EHE1}\)’ is the probability of field associated tunneling from ‘\(E_{AH}\)’ to ‘\(E_1\)’.

\[
P_{EHE1} = a(m^{1/8} / m^{*1/8})E_{AH}^{5/8} F_i^{1/4} \exp(-(b(m / m^*)^{-1/2} E_{AH}^{3/2}) / F_i) \]

................................. (38)

**Rate Equation 5:**

At time \(t=t_2\), the dipole (created by the electron in the bulk trap and the hole in the activator) collapses due to the reduction in net field and the rate at which they relax is given by

\[
R_5 = n_2\sigma_5(E) / \Delta t \quad \text{if } nt2 <= (u_0-u(x,t)-e(x,t)) \quad ........... (39a)
\]
\[
R_5 = (u_0 - u(x,t) - e(x,t))\sigma_5(E) / \Delta t \quad \text{if } nt2 > (u_0-u(x,t)-e(x,t)) \quad ...........(39b)
\]

Where, \(\sigma_5(E) = 1\), if \(F_i <= 1.1 \text{ MV/cm}\)
\(= 0\), if \(F_i > 1.1 \text{ MV/cm}\)

Where, ‘\(n_2\)’ is the trap density; ‘\(\Delta t\)’ is the time taken for dipole to collapse (= 50ns for simulation).

**Rate Equation 10:**

*Charge Transfer between the Conduction Band and Trap Level*

\[
R_{10} = n_2 P_{E1EC} \quad ................. (40)
\]

Where, ‘\(n_2\)’ is the concentration of electrons in the traps; ‘\(P_{E1EC}\)’ is the probability of field assisted tunneling from ‘\(E_1\)’ to ‘\(E_C\)’ and is given by,

\[
P_{E1EC} = a(m^{1/8} / m^{*1/8})E_{1C}^{5/8} F_i^{1/4} \exp(-(b(m / m^*)^{-1/2} E_{1C}^{3/2}) / F_i) \]

................................. (41)

Where, ‘\(E_{1C}\)’ is the energy gap between ‘\(E_1\)’ and ‘\(E_C\)’.

**Rate Equation 7:**

The rate of recombination from the conduction band to bulk traps is given by:

\[
R_7 = \left(\frac{f}{v_{SAT}}\right)p_T(i)S_m v_{TH} \quad ................. (42)
\]

Where, ‘\(v_{SAT}\)’ is the saturation velocity of electrons in the conduction band (\(cm/sec\)) (= 1 x 10^7 cm/sec); ‘\(f\)’ is the electron flux; ‘\(p_T(i)\)’ is the concentration of unoccupied trap levels; ‘\(v_{TH}\)’ is the thermal velocity of electrons in phosphor (\(cm/s\)) (= 23.3 x 10^6 cm/sec); ‘\(S_m\)’ is the capture cross-section area for recombination of electrons (\(cm^2\)) (= 1 x 10^{-16} cm^2).
The charge transfer between the ionized activators and shallow anodic interface states is modeled by the following rate equations.

\[ R_6 = (u_0 - u(x,t) - e(x,t)) \sigma_6(E) U(t - t_2) / \Delta t, \text{ if } (u_0 - u(x,t) - e(x,t)) < n_{AIS} \]  \hspace{1cm} (42a)

\[ R_6 = n_{AIS} \sigma_6(E) U(t - t_2) / \Delta t, \text{ if } (u_0 - u(x,t) - e(x,t)) > n_{AIS} \]  \hspace{1cm} (42b)

such that \( R_5 < n_e / \Delta t. \)

Where ‘\( \sigma_6(E) \)’ is the transition parameter and ‘\( n_{AIS} \)’ is the number of electrons tunnel ejected from the shallower anodic interface states.

\[ U(t-t_2) = 0 \text{ if } t < t_2 \]

\[ = 1 \text{ if } t > t_2 \]  \hspace{1cm} (43)

Where ‘\( t_2 \)’ is the time when the voltage pulse goes downward and the field direction reverses.

**Rate of change in the population of lower energy level of the activators:**

From Figure 3.1, we see that the overall electron transfer from lower energy level (\( E_{AL} \)) of the activator in the phosphor layer is given by:

\[ \frac{du(i)}{dt} = -R_1 + R_4 - R_2 - R_3 \]  \hspace{1cm} (44)

**Rate of change in the population of higher energy level of the activators:**

The overall electron transfer to the upper energy level (\( E_{AH} \)) of the activator in the phosphor layer is given by

\[ \frac{de}{dt} = R_5 - R_4 + R_9 + R_1 - R_{i2} - R_{i3} + R_6 \]  \hspace{1cm} (45)

**Rate of change in the population of traps:**

Similarly, net electron transfer to the trap level is given by

\[ \frac{dn_{i2}(i)}{dt} = R_7 - R_5 + R_2 - R_{i0} + R_{i1} + R_{i2} \]  \hspace{1cm} (46)
**Change in the flux population across the phosphor:**

For the purpose of numerical analysis, the phosphor layer is divided onto \( n \) subsections of “very small” width \( W_x \) each. Flux variation from one subsection \( (i-1) \) to the next subsection \( (i) \) can be expressed as

\[
 f(i) = f(i-1) + W_x \left[ R_{10} + R_{11} + R_3 + R_{13} - R_7 - R_9 \right]
\]  

\[\vdots\quad \text{……….. (47)}\]

Where ‘\( f(i) \)’ is the electron flux in the conduction band of host material.

These equations are used to calculate field, current and luminance in SrS:Cu ACTFEL devices.

The typical luminance output of SrS:Cu device is shown in Figure 3.2.

![Luminance vs Time](image)

**Figure 3.3:** **Typical luminance output of SrS:Cu device for the excitation voltage pulse shown in Figure 2.2.**

The luminance output of SrS:Cu exhibits three peaks namely the leading edge (LE), beginning of trailing edge (BTE) and the middle of trailing edge (MTE) as shown in Fig 3.2.

The various processes that are attributed to the peaks are impact excitation, impact ionization, dipole collapse and recombination of electrons and holes near the interfaces (described by the Physical Model in Section 2.2 and the expressions in Section 3.2).
The luminance output of section ‘i’ of phosphor in the time interval ‘Δt’ is,

\[ L(i,t) = Bn_{ai}(t)W_xΔτ_2 \] ....................... (48)

After summing the light output from all the sections, the total luminance is obtained as,

\[ L(t) = \sum L(i,t) \text{ where } i = 1,2,…,n \] ....................... (49)

### 3.4 Electron Capture at Interfaces

Electron flux (generated by tunneling from the interface states) travel through the phosphor. Due to impact ionization of the activators at each section of the phosphor, electrons leave the activators and add to the flux flowing through the phosphor. The electrons that reach the interface are trapped at the shallow interface states. These electrons at the shallow interface states then relax to the deeper interface states. The expression for this relaxation to deeper states is given by:

\[ dns_{ddt} = n_{SA} * Snd * Vth * (N_{states\_ad} - n_{DA}) \] ....................... (50)

\[ dnsdt = Fn[n] - dns_{ddt} \] ....................... (51)

\[ dnddt = dns_{ddt} \] ....................... (52)

\[ n_{SA} = n_{SA} + (dnsdt*delta_T) \] ....................... (53)

\[ n_{DA} = n_{DA} + (dnddt*delta_T) \] ....................... (54)

Where ‘dnsdt’ is the rate of change of population of the shallow interface state; ‘dnddt’ is the rate of change of population of the deep interface state; ‘dns_{ddt}’ is the rate at which the electron relaxes from the shallow to the deeper interface state; ‘delta_T’ is the relaxation time; ‘Fn[n]’ is the flux at the anodic interface; ‘n_{SA}’ is the number of electrons at the shallow anodic interface state; ‘n_{DA}’ is the number of electrons at the deeper anodic interface state; ‘S_{nd}’ is the surface recombination area and ‘V_{th}’ is the surface recombination velocity of electrons; ‘N_{states\_ad}’ is the number of states at the deeper anodic interface.

Similarly, the electrons in the shallow states at the cathodic interface relax from the shallow to the deeper interface states and the expressions are similar to those given above. The expressions are:

\[ dns_{ddt} = n_{SC} * Snd * Vth * (N_{states\_cd} - n_{CD}) \] ....................... (55)

\[ dnsdt = Fn[0] - dns_{ddt} \] ....................... (56)

\[ dnddt = dns_{ddt} \] ....................... (57)
\[ n_{SC} = n_{SC} + (d_{nsdt}\cdot\delta_T) \]  \hspace{1cm} \text{................. (58)}

\[ n_{DC} = n_{DC} + (d_{nddt}\cdot\delta_T) \]  \hspace{1cm} \text{................. (59)}

Where ‘d_{nsdt}’ is the rate of change of population of the shallow interface state; ‘d_{nddt}’ is the rate of change of population of the deep interface state; ‘d_{ns_{ddt}}’ is the rate at which the electron relaxes from the shallow to the deeper interface state; ‘\delta_T’ is the relaxation time; ‘F_{n[0]}’ is the flux at the cathodic interface; ‘n_{SC}’ is the number of electrons at the shallow cathodic interface state; ‘n_{DC}’ is the number of electrons at the deeper cathodic interface state; ‘S_{nd}’ is the surface recombination area and ‘V_{th}’ is the surface recombination velocity of electrons; ‘N_{states_{cd}}’ is the number of states at the deeper states of the cathodic interface.
Chapter 4

EXPERIMENTS

Experiments were performed by applying voltages of varying amplitudes and rise times to a SrS:Cu ACTFEL device and the results were plotted and stored. This chapter describes the equipments and software used to test and characterize ACTFEL devices and explains the experimental procedures adopted towards this end. The purpose of characterization was to obtain the following waveforms: Voltage applied to the device, Charge flowing through the device and the Luminance output from the device. These curves, collectively known as V-I-L curves, served as the starting point to analyze device operation.
4.1 Displays Testing System Hardware

The schematic of the Displays Testing System Hardware is shown in Figure 4.1.

![Schematic of Displays Testing System Hardware](image)

**Figure 4.1: Schematic of Displays Testing System Hardware**

A brief description of each instrument and component shown in the schematic is given below:

1. **Arbitrary Waveform Generator (SONY/Tektronix AWG 2005):**
   The AWG allowed us to generate the different waveforms that were applied to the device. The AWG could generate standard as well as custom waveforms from equations. A trapezoidal voltage was generated and was output through Channel 1. The maximum voltage that could be output from the AWG was 10V [5].

2. **Amplifier (Apex PA 89):**
   The ACTFEL device required a voltage in excess of 120V to operate, but, the maximum output voltage from the AWG was 10V. Hence, an amplifier was used to apply the desired voltage to the device. A variable potentiometer was used to set the gain of the amplifier [5].
3. Power Supplies (KEPCO APH 500M):

In order that the amplifier worked, suitable operating voltages had to be supplied to it. Two power supplies were used for this purpose. These two power supplies were capable of supplying +500V and -500V respectively. By using these two power supplies in Master/Slave configuration, it was ensured that the Slave power supply automatically tracked a change in the voltage supplied by the Master power supply. Since the output voltage of the amplifier did not exceed 160V during normal operation, voltages of +200V and -200V were supplied from the two power supplies to the amplifier [5].

4. Photo Multiplier Tube:

The light emitted by the device was collected by means of an optical cable. The light, so collected, was fed to a photomultiplier tube. It consisted of a photocathode and a series of dynodes in an evacuated glass enclosure. Photons that struck the photo emissive cathode emitted electrons due to the photoelectric effect. These electrons were accelerated towards a series of additional electrodes called dynodes. These electrodes were each maintained at a more positive potential. Additional electrons were generated at each dyode. This cascading effect created $10^5$ to $10^7$ electrons for each photon hitting the first cathode depending on the number of dynodes and the accelerating voltage. The amplified signal was finally collected at the anode and was measured [5].

5. Digital Storage Oscilloscope (Tektronix TDS 540D):

The Digital Storage Oscilloscope displayed and measured the electrical signal that was applied to it. Four inputs, namely, driving voltage to the device, voltage on the sense capacitor, output of the photomultiplier tube and current flowing through the device were given to the DSO [5].

6. PC:

The PC was used to control the operation of the instruments shown in the schematic above. The AWG and the DSO were connected through a GPIB cable to the GPIB interface card in the computer. The computer synchronized and controlled the operation of the equipments [5].

The devices used for characterization were obtained from Planar Inc., Finland.
The layout of a typical ACTFEL device that was characterized is shown below:

![Device Layout Image]

**Figure 4.2: Typical Device Layout**

A layer of ITO was coated on a glass substrate. The insulator layer, made up of ATO of thickness 0.16 µm, was deposited on the ITO layer. The phosphor layer (about 0.67µm) was deposited on top of the ATO layer. Another insulator layer, made up of BTO of thickness 0.22 µm, was deposited on top of this phosphor layer. Aluminum dots of diameter 1/8” were deposited on this insulator layer. Thus, many ACTFEL devices were made available on a single substrate.

Spring loaded probes were used to make contacts to the device. In order to make contacts to the ITO layer, a paste of a conducting metal was applied on top of the ITO layer. One probe was placed on the paste to make a contact. Another probe was placed over the top aluminum electrode to realize the second contact.

To measure the charge transferred across the ACTFEL device, a sense capacitor was placed between the ACTFEL device and the ground. The capacitance of this sense capacitor was 100 times greater than the total capacitance of the ACTFEL device, so that the voltage drop across the sense capacitor was negligible when compared to the voltage drop across the ACTFEL device [5].

### 4.2 Displays Testing System Software

The Displays Testing System software was developed in Labview 6.0 graphical programming environment. The software was designed to control the hardware, initiate the
measurements and record the generated data. The software generated the required waveforms in the Arbitrary Waveform Generator, adjusted its amplitude according to the gain of the amplifier (which it calibrated each time the measurements were performed), and acquired the voltage applied to the device, voltage across the sense capacitor, current flowing through the device and the light emitted by the device from the Digital Storage Oscilloscope. The data so obtained was displayed and stored in a text file, if necessary [5].

A snapshot of the front panel of Displays Testing System software is shown below:

![Figure 4.3: Display Testing System Front Panel.](image)

The software provided for 3 modes of operation, namely, Constant Voltage Mode, Voltage Sweep Mode and Wavelength Sweep Mode. A brief description of operation in all these modes is given below:
4.2.1. Constant Voltage Mode

Upon executing the program in ‘Constant Voltage Mode’, a preset number of voltage pulses of constant amplitude and rise and fall times were applied to the device. The parameters of the voltage applied to the device were input in the text fields provided in the tab titled ‘Constants’. Transient as well as steady state measurements could be taken when the program was executed in this mode. Figure 4.4 shows a snapshot of the Constants tab [5].

![Constants Tab of Displays Testing System Software](image)

**Figure 4.4:** Constants Tab of Displays Testing System Software

4.2.2. Voltage Sweep Mode

Upon executing the program in ‘Voltage Sweep Mode’, a preset number of voltage pulses of varying amplitude and rise and fall times were applied to the device. The parameters of the voltages applied to the device were input in the text fields provided in the tab titled ‘Voltage Sweep’. Figure 4.5 shows a snapshot of the Voltage Sweep tab [5].
4.2.3. Wavelength Sweep Mode

Upon executing the program in ‘Wavelength Sweep Mode’, the wavelength setting on the monochromator was adjusted and two sets of waveforms were recorded. The first set of waveforms was recorded by exciting the device with a low voltage which ensured that the device did not emit any light. Thus, light collected by PMT was composed of the light present in the background only. The second set of waveforms was recorded by exciting the device with the voltage necessary to produce light from the device. The light collected by the PMT now had two components: light emitted by the device and light present in the background. The background light was subtracted from the total light and the resultant light was integrated over many pulses to determine the light emitted by the device at a certain wavelength [5].
In addition to the three tabs shown above, another tab titled ‘Option’ was available. The Options tab provided the options to change the settings for the Arbitrary Waveform Generator, Digital Storage Oscilloscope and the Amplifier. Figure 4.6 shows a snapshot of the Options tab.
4.3. Experimental Procedure:

The procedure followed to obtain experimental VIL characteristics is outlined below:

1. The ACTFEL device was placed in the lab stand.
2. The spring loaded probes were used to make contacts to the metal electrodes in the ACTFEL device.
3. The two power supplies, waveform generator, PMT and the oscilloscope were switched ON.
4. The voltage applied to the amplifier was set to +200V and -200V using the two Master/Slave power supplies.
5. The supply voltage to the PMT was set to -1000V.
6. The output file, i.e. the file into which the voltage input to the device, the light emitted from the device and the charge flowing through the device was selected.
7. To record data for single/multiple pulses of voltage with a constant amplitude, the following steps were performed:
   i. The “Constants” tab was chosen.
   ii. The various parameters of the pulse, viz. Rise Time, Fall Time, On Time, Amplitude, Half Period, No. of Pulse Cycles, Transient Wait Time, Notch Start Time, Notch Length and Notch Depth were chosen depending on the experiments that needed to be performed and input into the appropriate text boxes.
   iii. The program was executed by clicking the ‘Run’ button in the menu bar.
   iv. Once the program indicated that the measurements had been recorded, the power supplies were switched off.

8. To record data for single/multiple pulses of voltage with varying amplitudes, the following procedure was adopted:
   i. The values were input into the fields in “Constants” tab that described the voltage pulse applied to the device.
   ii. The “Voltage Sweep” tab was chosen.
   iii. The starting voltage, final voltage, number of steps and the voltage step were chosen depending on the experiment to be performed and input into appropriate text boxes.
   iv. The program was executed by clicking the Run button in the menu bar.
   v. Once the program indicated that the measurements had been completed, the power supplies were switched off.
Chapter 5
SIMULATIONS

Simulations were carried out to verify the accuracy of the model developed to describe the optoelectronic processes in the phosphor. Section 5.1 details the procedure used to simulate the analytical model. Section 5.2 provides a brief description of the routines, variables and constants used in the simulation program. A flow chart, that describes the procedure used for simulations, is given in Section 5.3.
5.1 Simulation Procedure

In order to numerically simulate the optoelectronic processes described in Section 2.3 and obtain the simulated luminance and flux waveforms, which are later compared with the experimentally obtained waveforms, a program was coded in C and run in a UNIX environment. The equations described in Chapter 3 were incorporated into the simulation program.

The simulation procedure adopted is described below:

1. The voltage applied to the device was increased in steps until its maximum value was attained. The voltage was held constant at this maximum value and then reduced to zero in steps. The duration of the voltage pulse was characterized by its rise, hold and fall times. The time increment (i.e. the time between successive voltage increments) was chosen to be 50ns, which was compatible with the sampling rate of our oscilloscope. It was assumed that the electric field in the device was constant in this 50ns interval. The step height was determined as the ratio of the maximum voltage to the rise or fall times depending on whether the voltage was rising to its maximum value or falling to zero.

2. The phosphor was divided into ‘n’ sections. The value of ‘n’ was chosen to be 10. This was an optimal value obtained as a tradeoff between accuracy and computation time.

3. The electric field in each of these ‘n’ sections was calculated by solving Poisson’s equation using appropriate boundary conditions. It was assumed that the electric field remained constant during each of the 50ns interval in each of these sections.

4. The flux of electrons that tunneled out of the interface states at both the cathode and anode, as a result of the electric field in the phosphor, was calculated according to the Fowler-Nordheim tunneling equations described in Section 3.2. The electron populations at both levels of the interface states were updated.

5. The flux was made to flow from the cathodic to the anodic interface if more electrons tunneled out of the cathodic interface; and, in the opposite direction, if otherwise.

6. The change in the population of the lower and higher energy levels of the activators and traps, as well as the flux of electrons in the conduction band was
calculated (using the rate equations described in Section 3.3). The flux of electrons that traveled to the next section was computed by adding the flux in the present section and the relevant rate equations (as described in equation 47 in Section 3.3). The resulting flux initiated the optoelectronic processes in the subsequent sections.

6. The luminance in each section was computed (using Equation 48 in Section 3.3) and the total luminance was computed by summing up light emitted from each section (using Equation 49 in Section 3.3).

7. The flux in the final section was trapped at the shallow state at the phosphor-insulator interface; the flux, subsequently, relaxed to the deep state.

8. Steps 3 to 7 were repeated, with the voltage “built” as described in Step 1.

9. In order to obtain results at steady state, steps 1 to 9 were repeated for several pulses. If simulations were required to run for alternating positive and negative voltage pulses, the following procedure was adopted:
   a. The states of the two interfaces were interchanged.
   b. The state of the activators and traps in the k\textsuperscript{th} section was exchanged with that in the (n-k)\textsuperscript{th} section where ‘k’ varied from 1 to ‘k/2’.

10. Steps 1 to 9 were repeated for the desired number of pulses.

11. The results obtained, namely the voltage applied to the device, electric field in various sections, flux in the phosphor and luminance were saved in separate data files. The results were plotted using Microsoft Excel.

For the program listing, refer Appendix.

5.2 Simulation Program

The program was coded in 3 files, namely prog.c, constants.h and variables.h. A brief explanation of the routines in the file prog.c, in which the optoelectronic processes were described, is given below.
The processes described in Section 5.1 were encoded in the file `prog.c`. The program was divided into many modules and specific processes were coded in each module. The various subroutines in the program are listed below along with a description of the processes performed in these routines:

a. **main( )**

The ‘main( )’ routine was executed first when the program was compiled and run. The data files, into which the values of driving voltage, electric field, luminance, flux etc. were written at the end of each $\Delta t$, were opened. Then, the function `init()` was called. Upon execution of the function `init()`, the control was transferred back to `main()`. The simulations were run for multiple pulses of the driving voltage, if necessary. Function calls to `driver()` and `anodic_interface()` were performed. The subroutine `exchange()` was called if the simulations were needed to be performed for multiple alternating voltage pulses. Upon executing these routines for the desired number of pulses, all data files were closed.

b. **init( )**

The `init( )` routine was used to initialize the values of certain variables used for simulations. These variables included the electron density in the excited (higher) energy level of the activator (which was initialized to zero), the trap level (which was initialized to zero) and the lower energy level of the activator (which was initialized to contain all the electrons within the activator atoms). Additionally, the electron density at the shallow anodic and cathodic interface states were initialized to zero and their densities at the deep state were initialized to their equilibrium values.

c. **driver( )**

The ‘driver( )’ routine was used to “build” the voltage pulse. i.e. the pulse was slowly built to its maximum value depending on the rise time, held steady at
the maximum value as determined by its hold time and reduced to zero depending on the fall time. The step width (Δt) was chosen to be 50ns. Then, the calls to the functions `constants()`, `cathodic_interface()` and `bulk_phosphor()` were implemented, in that order. Upon executing these functions, the control was transferred back to the `driver()` routine. The values of the driving voltage, electric field and flux were written into the files opened in the `main()` routine. The luminance in each section was added and the total luminance for that time interval was written into the luminance data file.

d. **constants()**

The ‘`constants()`’ routine was used to calculate the value of the electric field in each of the ‘n’ sections of the phosphor (using the equations described in Section 3.1). The local electric field in each section was stored in an array named ‘c3’. The array index referred to the section. The values of the electric field in the cathode, anode as well as any other sections of interest were written into the data files in this routine.

e. **cathodic_interface()**

The ‘`cathodic_interface()`’ routine was used to calculate the flux of electrons tunneling out of the cathodic interface (the interface between the phosphor and the insulator Al₂O₃) by Fowler-Nordheim tunneling. The probabilities of tunneling from the various interface states was calculated for a given field at the cathode. The flux from each interface state was calculated by multiplying the probabilities of tunneling from each interface state by the density of electrons in that interface state. The total flux in the first section was computed by adding the flux from every interface state. The population of the interface states was updated to reflect the change in population due to the flux tunneling out of the interface.
f. \textit{anodic\_interface()} \\
The ‘anodic\_interface( )’ routine was called when the net field (defined as the difference between the applied electric field and the internal field) at the anode became negative. The flux of electrons tunneling out of the anodic interface (the interface between the phosphor and the insulator Ba$_2$TaO$_6$) was calculated in this routine. The electrons tunneled out of the anodic interface due to the applied electric field by Fowler-Nordheim tunneling. The probabilities of tunneling from the various interface states was calculated for the net field at the anode. The flux from each interface state was calculated by multiplying the probabilities of tunneling from each interface state by the density of electrons in that interface state. Then, the total flux was computed by adding all the flux from the interface states. The population of the interface states was updated to reflect the change in population due to the flux tunneling out of the interface.

g. \textit{bulk\_phosphor()} \\
The ‘bulk\_phosphor( )’ routine was used to describe the optoelectronic processes taking place in the phosphor. The luminance contribution of each section was calculated. The rate equations (described in Section 3.2) were used to calculate the change in the population of electrons in the lower and higher energy levels of the activator and the bulk trap. The flux that had initiated the optoelectronic processes in the current section was added to the flux generated in the section under consideration and the resulting flux caused the optoelectronic processes in the next section. The direction of flow of flux was chosen to be from cathode to anode if the number of electrons tunneling from the cathode was larger than the number of electrons tunneling from the anode and from anode to cathode, if otherwise.
h. **anodic_interface()**

The ‘anodic_interface( )’ routine was used to trap the flux flowing toward the anode in the shallow state of the anodic interface. The electrons at the shallow anodic interface state were then made to relax to the deep anodic interface state (as described by the equations in Section 3.4).

i. **cathodic_interface()**

The ‘cathodic_interface( )’ routine was used to trap the flux flowing toward the anode in the shallow state of the cathodic interface. The electrons at the shallow cathodic interface state were then made to relax to the deep cathodic interface state (as described by the equations in Section 3.4).

j. **exchange()**

The ‘exchange( )’ routine was used to enable the simulations to be executed for multiple driving voltage pulses (where pulses alternated as positive and negative) using the same subroutines described above. However, in order to do so, the state of the k\(^{th}\) section in the phosphor was swapped with the (n-k)\(^{th}\) section of the phosphor (k varied between 1 to n/2). The electron densities at the shallow and deep states of the cathodic and anodic interfaces were also swapped.

2. **constants.h**

The values of constants used during simulations were defined in the file “constants.h”. These constants included the

a. attributes of the driving voltage like the amplitude ($V_{max}$), half pulse width ($T_s$), rise time ($RISE\_TIME$) and fall time ($FALL\_TIME$),
b. time interval for simulations ($\Delta t$), taken as 50ns,
c. number of sections ($n$), taken as 100,
d. number of pulses for which the simulation were needed to run ($NO\_OF\_PULSES$),
e. depth of various energy levels from the conduction band \((E_1, E_{11}, E_{AL}, E_{AH}, E_T)\),
f. device parameters such as the density of activators in phosphor \((N_{ao})\), the densities of interface states \((n_{c1}, n_{c1l}, n_{d1}, n_{d1l})\), the dielectric constants \((e_s, e_d)\) and the device dimensions \((W_z, W_x)\),
g. various physical constants such as the mass of an electron \((m)\), charge of an electron \((q)\) and the luminance output for electron transitions between higher and lower energy levels \((B)\) and
h. values of the various parameters used in the equations describing the rates of transitions between various energy levels.

3. **variables.h**

The variables used in the simulation program were declared in the file “variables.h”. These variables included

a. file pointers that referred to the various output data files which stored the data obtained during the simulation runs,
b. rate variables that stored the different rates as described by the mathematical model for each time increment,
c. variables that stored the values of flux, number of electrons in the activators, traps and interface states,
d. variables that stored the values of the space charge and the activator charge,
e. variables used during the calculation of electric field by the bisection method, and
f. variables that stored the temporary values of various parameters in the rate equations.
5.3 Simulation Flowchart

Start

Open data files to store results of simulations

1. The electrons at interface states are at shallowest level.
2. The electrons are at lower energy level within activator.
3. There are no electrons in traps.
4. Initialize time to zero.

Define and build voltage by amplitude, and rise and fall times.

Calculate electric field in all ‘n’ phosphor sections using equations 1 to 23 in chapter 3.

Write electric field at cathode, anode and mid-phosphor into data files.
1. Calculate probabilities of tunneling from shallow and deep cathodic interface states.
2. Calculate flux from both energy levels and add them up.
3. Update population at both energy levels.

- Is field at anode < 0?
  - NO: Flux travels from the cathodic interface towards anodic interface
  - YES: Calculate flux tunneling from anodic interface states and update population at anodic interface

- Is flux from anodic interface > flux from cathodic interface?
  - N: Calculate light output from single section
  - YES: Flux travels from the anodic interface towards cathodic interface

- Calculate rates of charge transfer between various energy levels according to equations 27 to 43 in Chapter 3.

- Update population at energy levels according to equations 44 to 46.
Calculate flux leaving the current section according to equation 47 in Chapter 3.

Trap flux at shallow energy level at cathodic or anodic interface depending on direction of flux flow and relax to deep state.

Increment time by 50 ns

Has simulation been performed for entire duration of driving voltage pulse?

Yes

Should simulations be executed for multiple voltage pulses of alternating polarity?

Yes

1. Exchange states of anodic interfaces
2. Exchange population in activators and traps in k\textsuperscript{th} section with those in (n-k)\textsuperscript{th} section; ‘k’ varied from 1 to ‘n/2’

Stop
Chapter 6

COMPARISON OF EXPERIMENTAL AND SIMULATED RESULTS

Experimentally obtained VIL characteristics are compared with simulated VIL characteristics in this chapter. A comparison of experimental and simulated VIL characteristics for different driving voltages is performed in Section 6.1; similar comparisons are performed for different rise and fall times in Section 6.2. The depth of energy levels of shallow and deep interface states from conduction band is varied during simulations and results are discussed in Section 6.3. The electric field at which the dipoles collapse is varied and the results are discussed in Section 6.4. The number of traps in the phosphor is varied and results are presented in Section 6.5.
Section 6.1: Comparison of Experimental and Simulated VIL Waveforms for Different Driving Voltages

6.1.1. Procedure:

Voltage pulses of varying amplitude were applied to the device and different sets of data were collected. Simulations were performed by applying different voltages to the device and the data on the resulting flux and luminance was collected for each of these voltages. The results were plotted using MATLAB. VIL characteristics were plotted for each of these voltages.
6.1.2. Results and Discussion:

The experimental and simulated VIL characteristics for driving voltages of 120V, 140V and 160V are given below:

6.1.2.1: Driving Voltage = 120V

Experimentally obtained VIL characteristics are shown in Figure 6.1.1.1 and the simulated VIL characteristics are shown in Figure 6.1.1.2.

Figure 6.1.2.1.1: Experimentally obtained VIL characteristics for driving voltage of 120V with rise time and fall time of 100µs
Observations and Analysis:

1. The current reached its maximum value much earlier than voltage. It is attributed to the following processes occurring in the device:
   a. The electric field applied to the device increases as the voltage applied to the device increases.
   b. When the threshold electric field for tunneling from interface states is reached, electrons tunnel out of the insulator-phosphor interface and reach the other interface.
   c. On their path, the electrons collide with the activators and ionize them. As a result, there is a positively charged interface (from which the electrons have tunneled out), positively ionized activators in the bulk of the phosphor (ionized upon impact by the hot electrons) and a negatively charged interface (as a result of trapping the electron flux). Hence, an internal electric field builds up in the phosphor and the direction of this internal field is opposite to the direction of the applied electric field. The rate of increase of internal electric field is dependent upon the rate at which flux is ejected from the interface, the rate at which impact ionization occurs in the phosphor and the rate at which electron is transferred from one interface to another.
   d. When the rate of increase of internal electric field is greater than the rate of increase of applied electric field, the net electric field in the phosphor decreases (despite the increasing driving voltage). This decrease in the net electric field decreases the flux of electrons tunneling out of the interface and reduces the number of electrons tunneling out into the conduction band of the phosphor. Since the number of electrons tunneling out of the interface is proportional to the net field present in the phosphor, the flux peaks when the net electric field in the phosphor is greatest; the net electric field reaches its maximum much before the driving voltage reaches its maximum value.

2. The luminance exhibits a leading edge peak (labeled LE, for Leading Edge) with a shoulder, a peak when the driving voltage begins to decrease (labeled BTE, for Beginning of Trailing Edge) and a third peak when the driving voltage has almost fallen to zero (labeled MTE, for Middle of Trailing Edge). The leading edge peak is due to
excitation and relaxation processes within the Cu activator; the shoulder in the LE peak and the BTE peak are produced when the dipoles in the bulk collapse; and the MTE peak is caused when the ionized activators recapture the electrons that tunnel from the anodic interface states (For more details, refer Section 2.3).

3. On observing the VIL characteristics, we find that the luminance reached its maximum value much earlier than current did. This is explained in terms of saturation of activators:
   a. The flux ejected from the interface impacts the Copper activators causing excitation and ionization processes. The excitation process is followed by relaxation within the Copper activator.
   b. Assuming that the initial fraction of electron flux that impacts the activators is ‘x’, the number of activators present is ‘y’ and the fraction of electrons impact ionized is ‘z’ and impact excited is ‘1-z’ (assuming that an impact causes either an excitation or ionization process), the total number of activators impact excited is ‘x.y.(1-z)’ and the total number of activators impact ionized is ‘x.y.z’.
   c. The number of remaining unionized activators is ‘y-(x.y.z)’.
   d. The percentage increase in electron flux after impact ionization is ‘(x+x.y.z)/x = 1+y.z’; thus, flux increases with each impact.
   e. The number of activators available for impact decreases with each impact process.
   f. Thus, at some later time, no unionized activators are available for impact. Hence, any subsequent increase in flux has no effect on the light emitted by the device.
   g. Consequently, luminance reaches its maximum value much before current does and begins to decrease even though current increases.
Figure 6.1.2.1.2: Simulated VIL characteristics for driving voltage of 120V with rise time and fall time of 100µs

Observations and Analysis:

1. The flux is made up of two components: displacement flux and conduction flux.
   a. The displacement flux is given by,
      
      \[
      \text{Displacement Flux} = C \frac{dV}{dt}
      \]
      
      Where, \(dV/dt\) is the rate of change of driving voltage with respect to time and \(C\) is the total capacitance of the device.

      The total capacitance of the device is calculated by considering the device to be made up of 3 capacitors in series, as shown in Figure 6.1.2.1.2.1.

      \[
      \begin{align*}
      & - C_{11} \quad \text{C}_P \quad \text{C}_{12} \quad +
      \end{align*}
      \]

      Figure 6.1.2.1.2.1: Equivalent diagram of an ACTFEL device
Equivalently, the 3 capacitors are represented as a single capacitor with total capacitance ‘C’.

![Diagram of capacitors](image)

**Figure 6.1.2.1.2.2: Equivalent diagram of an ACTFEL device with the three capacitors in series replaced by a single capacitor**

The value of C is given by,

\[
C = \frac{(C_{I1} \cdot C_{I2}/(C_{I1}+C_{I2})) \cdot C_P}{((C_{I1} \cdot C_{I2}/(C_{I1}+C_{I2})) + C_P)}
\]

b. The other component of flux is the conduction flux, which begins to flow once the driving voltage reaches the threshold voltage of the device. As can be seen from Figure 6.1.2.1.2, the threshold voltage is approximately 30V. The flux attained its maximum value much before voltage did, as in experiments.

i. This is attributed to the internal electric field setup in the device, as a result of transfer of charges across the interface and generation of space charge in the phosphor. The net electric field varies spatially across the device. The net electric field at the anode is much less than the net electric field at the cathode. The impact of spatial variation in electric field on the VIL characteristics is discussed later in the chapter.

2. The luminance waveform exhibited two peaks: Leading Edge (LE) and Beginning of Trailing Edge (BTE) peaks.

   a. The flux peaked much earlier than LE luminance.
      i. This is because it takes a finite time for electrons to relax from the higher to the lower energy level within the activator.

   b. The BTE luminance did not exhibit a single smooth rise and fall curve like leading edge luminance did; instead it was made up of several closely spaced peaks.
i. The jagged BTE waveform is attributed to spatial variation of electric field within the phosphor.

ii. The BTE luminance is produced due to the collapse of dipoles, and subsequent relaxation of the electron within the activator. The time of collapse is determined by the time at which the net electric field in the phosphor goes below a threshold field. For the purpose of simulations, the phosphor was divided into 100 sections. The electric field varied spatially across the sections. Hence, the dipoles collapse at different instances of time in different sections in phosphor. As a result, we get many closely spaced peaks. This is explained in detail in Section 6.4.

c. The MTE luminance was produced when the net electric field in the phosphor reversed its direction.
6.1.2.2: Driving Voltage = 140V

Experimentally obtained VIL characteristics are shown in Figure 6.1.2.1 and the simulated VIL characteristics are shown in Figure 6.1.2.2.

![Experimental VIL characteristics for V = 140V](image)

Figure 6.1.2.2.1: Experimentally obtained VIL characteristics for driving voltage of 140V with rise time and fall time of 100µs

**Observations and Analysis:**

1. It is observed from Figure 6.1.2.2.1 that the current reached its maximum value much before the voltage reached its maximum.
2. The luminance exhibits a leading edge (LE) peak with a shoulder, a peak when the driving voltage begins to decrease (BTE) and a third peak when the driving voltage has almost fallen to zero (MTE).
3. The luminance reached its maximum value much earlier than current did.

These observations are explained in Section 6.1.2.1.1.
Figure 6.1.2.2: Simulated VIL characteristics for driving voltage of 140V with rise time and fall time of 100µs

Observations and Analysis:

1. The flux peaked much earlier than LE luminance.
2. The luminance waveform exhibited three peaks: Leading Edge (LE), Beginning of Trailing Edge (BTE) and Middle of Trailing Edge (MTE) peaks.
3. The BTE luminance did not exhibit a single smooth rise and fall curve like leading edge luminance did; instead it was made up of several closely spaced peaks.
4. The MTE luminance was produced due to the recapture of electrons tunneling from the anodic interface states (caused due to reversal of electric field in the phosphor) by the ionized activators in its vicinity.
6.1.2.3: Driving Voltage = 160V

Experimentally obtained VIL characteristics are shown in Figure 6.1.3.1 and the simulated VIL characteristics are shown in Figure 6.1.3.2.

![Applied Voltage, Current and Luminance vs. Time](image)

**Figure 6.1.2.3.1:** Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs

**Observations and Analysis:**

1. It is observed from Figure 6.1.2.3.1 that the current reached its maximum value much before the voltage reached its maximum.

2. The luminance exhibits a leading edge (LE) peak with a shoulder, a peak when the driving voltage begins to decrease (BTE) and a third peak when the driving voltage has almost fallen to zero (MTE).

3. The luminance reached its maximum value much earlier than current did.

These observations are explained in Section 6.1.2.1.
Figure 6.1.2.3.2: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs
Figure 6.1.2.3.3: Simulated BTE luminance for driving voltage of 160V with rise time and fall time of 100µs

1. The flux peaked much earlier than LE luminance.
2. The luminance waveform exhibited three peaks: LE, BTE and MTE peaks.
3. The BTE luminance did not exhibit a single smooth rise and fall curve like leading edge luminance did; instead it was made up of several closely spaced peaks (Figure 6.1.2.3.3). These observations are explained in Sections 6.1.2.1.2 and 6.1.2.2.2.
4. A number of smaller luminance peaks are observed between the LE and BTE luminance peaks. These small peaks are produced by the collapse of dipoles in the bulk. Further studies have been performed to investigate this phenomenon and the results are reported in Section 6.4.
Section 6.2: Comparison of Experimental and Simulated VIL Waveforms for Driving Voltages of Constant Amplitude and Different Rise and Fall Times

6.2.1. Procedure:

Experiments were performed by applying voltage pulses of constant amplitude (160V) and different rise and fall times to the device; the rise and fall times were varied from 30µs to 150µs and different sets of data were collected. Simulations were performed by applying voltages of constant amplitude (160V) and varying its rise and fall times from 30µs to 150µs and the data on the resulting flux and luminance was collected. The results were plotted using MATLAB. The experimental and simulated results are presented below:
6.2.2. Results:

6.2.2.1: Driving voltage = 160V; Rise Time = Fall Time = 30µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.1.1 and the simulated VIL characteristics are shown in Figure 6.2.1.2.

\[\text{Figure 6.2.2.1.1: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 30}\mu\text{s}\]

Observations and Analysis:

1. The conduction current flowed when the driving voltage was about 12V, for smaller rise times and the conduction current had fallen to zero by the time the voltage had reached its maximum value (Figure 6.2.2.1.1). This is reasoned out below:

   Since charges are transferred to the other interface rapidly, internal electric field builds up very quickly in the phosphor. At some instant much before the voltage reaches its maximum, the rate of increase of internal electric field is greater than the rate of increase of external field. Hence, the net electric field in the phosphor decreases, which results in fewer electrons tunneling out of the interface states.
Consequently, conduction current falls to zero by the time the driving voltage has reached its maximum value.

2. The luminance curves exhibited interesting characteristics. The LE luminance peaked slightly ahead of current. This is attributed to the saturation of activators and is explained in Section 6.1. There was a pronounced shoulder in the LE luminance. The cause for the shoulder in luminance peak is discussed in Section 6.1.

3. The BTE peak was clearly absent.

4. The MTE luminance peak was large and sharp. This is reasoned out below:
   a. The electrons are driven very quickly from the anodic interface states by a rapidly growing net electric field (since the driving voltage is decreasing rapidly).
   b. Hence, they recombine with the ionized activators and impact unionized activators more rapidly; subsequent relaxation of electrons within the activators produces a larger and sharper MTE.

Figure 6.2.2.1.2: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 30µs
Observations and Analysis:

1. The conduction current flowed when the driving voltage was about 20V (Figure 6.2.2.1.2).

2. The MTE luminance peak was sharp. This is reasoned out below:
   a. The electrons are driven very quickly from the anodic interface states by a rapidly growing net electric field (since the driving voltage is decreasing rapidly).
   b. Hence, they recombine with the ionized activators and impact unionized activators more rapidly; subsequent relaxation of electrons within the activators produces a sharper MTE.
   c. The shape of the MTE luminance could thus be controlled by changing the fall time of the driving voltage, the population at the interface states, the depths of the energy levels of the interface states and the time taken for relaxation from the shallow to the deeper interface states.
6.2.2.2: Driving voltage = 160V; Rise Time = Fall Time = 60µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.2.1 and the simulated VIL characteristics are shown in Figure 6.2.2.2.

![Experimental VIL characteristics for V = 160V](image)

**Figure 6.2.2.1:** Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 60µs

**Observations and Analysis:**

1. The conduction current flowed when the driving voltage was about 16V and the conduction current had fallen to zero by the time the voltage had reached its maximum value (Figure 6.2.2.2.1).

2. The luminance curves exhibited interesting characteristics. The LE luminance peaked slightly ahead of current. This is attributed to the saturation of activators and is explained in Section 6.1. There was a pronounced shoulder in the LE luminance. The cause for the shoulder in luminance peak is discussed in Section 6.1.

3. The magnitude of BTE luminance was less.
4. The MTE luminance peak was large and sharp, but not quite as sharp as in Figure 6.2.2.1.1. This is attributed to the greater fall time.

**Figure 6.2.2.2.2**: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 60µs

**Observations and Analysis:**

1. The conduction current flowed when the driving voltage was about 28V (Figure 6.2.2.2.2).
2. The MTE luminance peak was sharp.

These observations are explained in Section 6.2.2.1.2.
6.2.2.3: Driving voltage = 160V; Rise Time = Fall Time = 90µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.3.1 and the simulated VIL characteristics are shown in Figure 6.2.3.2.

![Experimental VIL characteristics for V = 160V](image)

**Figure 6.2.2.3.1:** Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 90µs

**Observations and Analysis:**

1. The conduction current flowed when the driving voltage was about 20V, for smaller rise times and the conduction current had fallen to zero by the time the voltage had reached its maximum value (Figure 6.2.2.3.1).

2. The luminance curves exhibited interesting characteristics. The LE luminance peaked before current peaked. This is attributed to the saturation of activators and is explained in Section 6.1. There was a pronounced shoulder in the LE luminance. The cause for the shoulder in luminance peak is discussed in Section 6.1.
3. Though the BTE peak was negligible, a bump in the luminance curve was noticed. The cause of this phenomenon is the same as the one that produces BTE luminance, namely collapse of dipoles in the phosphor.

Figure 6.2.2.3.2: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 90µs

Observations and Analysis:

1. The conduction current flowed when the driving voltage was about 28V (Figure 6.2.2.3.2).
2. The MTE luminance peak was sharp.
   These observations are explained in Section 6.2.2.1.2.
3. A number of small peaks are present between the LE and BTE luminance. These peaks are caused by the collapse of dipoles and are explained in Section 6.4.
6.2.2.4: Driving voltage = 160V; Rise Time = Fall Time = 100µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.5.1 and the simulated VIL characteristics are shown in Figure 6.2.5.2.

![Experimental VIL characteristics for V = 160V](image)

**Figure 6.2.2.4.1:** Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs

**Observations:**

1. The luminance curve exhibits three peaks: LE, BTE and MTE peaks (Figure 6.2.2.4.1).
2. A shoulder is present in the LE peak.
3. A bump is noticed between the LE and BTE peaks.
**Figure 6.2.2.4.2:** Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs

**Observations and Analysis:**

1. The conduction current flowed when the driving voltage was about 28V (Figure 6.2.2.4.2).

2. A number of small peaks are present between the LE and BTE luminance. These peaks are caused by the collapse of dipoles and are explained in Section 6.4.
6.2.2.5: Driving voltage = 160V; Rise Time = Fall Time = 110µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.5.1 and the simulated VIL characteristics are shown in Figure 6.2.5.2.

![Experimental VIL characteristics for V = 160V](image)

Figure 6.2.2.5.1: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 110µs

Observations:

1. The luminance curve exhibits three peaks: LE, BTE and MTE peaks (Figure 6.2.2.5.1).
2. A shoulder is present in the LE peak.
3. A bump is noticed in the luminance curve between the LE and BTE peaks.
Figure 6.2.2.5.2: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 110μs

Observations and Analysis:

1. A number of small peaks are present between the LE and BTE luminance (Figure 6.2.2.5.2). These peaks are caused by the collapse of dipoles and are explained in Section 6.4.
6.2.6.2: Driving voltage = 160V; Rise Time = Fall Time = 120µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.6.1 and the simulated VIL characteristics are shown in Figure 6.2.6.2.

![Experimental VIL Characteristics for V = 160V](image)

**Figure**

**6.2.2.6.1:** Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 120µs.

**Observations:**

1. The luminance curve exhibits three peaks: LE, BTE and MTE peaks (Figure 6.2.2.6.1).
2. A shoulder is present in the LE peak.
3. A bump is noticed in the luminance curve between the LE and BTE peaks.
Figure 6.2.2.6.2: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 120µs
6.2.2.7: Driving voltage = 160V; Rise Time = Fall Time = 130µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.7.1 and the simulated VIL characteristics are shown in Figure 6.2.7.2.

**Figure 6.2.2.7.1:** Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 130µs.
6.2.2.7.2: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 130µs
6.2.2.8: Driving voltage = 160V; Rise Time = Fall Time = 140µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.8.1 and the simulated VIL characteristics are shown in Figure 6.2.8.2.

Figure 6.2.2.8.1: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 140µs.
**Figure 6.2.2.8.2:** Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 140µs
6.2.2.9: Driving voltage = 160V; Rise Time = Fall Time = 150µs.

Experimentally obtained VIL characteristics are shown in Figure 6.2.9.1 and the simulated VIL characteristics are shown in Figure 6.2.9.2.

Figure 6.2.2.9.1: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 150µs.
**Figure 6.2.2.9.2**: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 150µs
6.2.3. Observations and Analysis:

1. The conduction current had fallen to zero by the time the voltage had reached its maximum value (Figs. 6.2.2.1 to 6.2.2.9.2). This is reasoned out below:
   
   Since charges are transferred to the other interface rapidly, internal electric field builds up very quickly in the phosphor. At some time instant much before the voltage reaches its maximum, the rate of increase of internal electric field is greater than the rate of increase of external field. Hence, the net electric field in the phosphor decreases, which results in fewer electrons tunneling out of the interface states. Consequently, conduction current falls to zero by the time the driving voltage has reached its maximum value.

2. The luminance curves exhibited interesting characteristics. The LE luminance peaked at almost the same time instant as the current peaked. There was a pronounced shoulder in the LE luminance. The cause for shoulder in the luminance peak is discussed in Section 6.1.

3. The BTE peak was clearly absent for shorter fall times.

4. The MTE luminance peak was larger and sharper for shorter fall times. This is reasoned out below:
   
   a. The electrons are driven very quickly from the anodic interface states by a rapidly growing net electric field (since the driving voltage is decreasing rapidly).
   
   b. Hence, they recombine with the ionized activators and impact unionized activators more rapidly; subsequent relaxation of electrons within the activators produces a larger and sharper MTE.
   
   c. The shape of the MTE luminance could thus be controlled by changing the fall time of the driving voltage, the population at the interface states, the depths of the energy levels of the interface states and the time taken for relaxation from the shallow to the deeper interface states.
Section 6.3: Changing Depth of Interface States

6.3.1. Procedure:

Theoretical studies were performed to determine the effect of varying the depth of interface states on the VIL characteristics. The depths of the cathodic and anodic interface states (with respect to the conduction band) were varied over a determined range of values and simulations were performed. The time taken for relaxation from the shallow to the deep interface states was negligible when compared to the time between successive voltage pulses; the time taken for relaxation from shallow to deep states was taken as 50ns and the time between successive voltage pulses was taken as 450µs. As a result, all electrons were present at the shallow state at the interfaces when the next voltage pulse was applied to the device.
6.3.2. Results:

Simulated VIL characteristics, obtained by varying depths of shallow and deep interface states, are presented below:

6.3.2.1: Depth of shallow interface state = 0.2eV; Depth of deep interface state = 0.5eV.

![Simulated VIL Characteristics for Driving Voltage of 160V with Depth of Shallow Interface State = 0.2 eV and Depth of Deep Interface State = 0.5 eV](image)

**Figure 6.3.2.1:** Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 140µs; Energy level of the shallow interface state = 0.2eV; Energy level of the deep interface state = 0.5eV.

**Observations and Analysis:**

1. The magnitude of the BTE luminance is large and it exhibits oscillations (Figure 6.3.2.1). The reason behind the presence of oscillations is described in Section 6.4.

2. The LE luminance exhibits a peak (Figure 6.3.2.1).

   A large number of electrons tunnel out of the deep interface states since the seep interface states are not very deep. Hence, at some time instant (before the voltage reaches its maximum), the magnitude and rate of increase of internal electric field is greater than the magnitude and rate of increase of the applied electric field. At this time instant, the flux and luminance curves exhibit well defined peaks.
3. Many smaller luminance peaks are observed between the LE and BTE luminance peaks. Since dipoles collapse at different times in different sections, such luminance peaks are observed. This has been explained in detail in Section 6.4 where the effect of varying the threshold field for dipole collapse on the BTE luminance is discussed.
6.3.2.2: Depth of shallow interface state = 0.3eV; Depth of deep interface state = 0.5eV.

**Figure 6.3.2.2:** Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 140µs; Energy level of the shallow interface state = 0.3eV; Energy level of the deep interface state = 0.5eV.

**Observations and Analysis:**

1. The magnitude of the BTE luminance is large and it exhibits oscillations (Figure 6.3.2.2). The reason behind the presence of oscillations is described in Section 6.4.

2. The LE luminance exhibits a peak (Figure 6.3.2.2).

3. Many smaller luminance peaks are observed between the LE and BTE luminance peaks. These observations have been explained in Section 6.3.2.1.
6.3.2.3: Depth of shallow interface state = 0.4eV; Depth of deep interface state = 0.5eV.

Simulated VIL Characteristics for Driving Voltage of 160V with Depth of Shallow Interface State = 0.4eV and Depth of Deep Interface State = 0.5eV

Figure

6.3.2.3: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 140µs; Energy level of the shallow interface state = 0.4eV; Energy level of the deep interface state = 0.5eV.

Observations and Analysis:

1. The magnitude of the BTE luminance is large and it exhibits oscillations (Figure 6.3.2.3). The reason behind the presence of oscillations is described in Section 6.4.

2. The LE luminance exhibits a peak (Figure 6.3.2.3).

3. Many smaller luminance peaks are observed between the LE and BTE luminance peaks. These observations have been explained in Section 6.3.2.1.

4. Figs. 6.3.2.1 to 6.3.2.3 show similar VIL characteristics. It leads us to conclude that the depth of shallow interface state does not play a major role in determining the VIL characteristics. However, it must be noted that during simulations, the electrons are allowed to relax from shallow to the deep interface states before the next voltage pulse is applied. Hence, the electrons would be present in the deep interface states when the next voltage pulse is applied.
6.3.2.4: Depth of shallow interface state = 0.4eV; Depth of deep interface state = 0.6eV.

![Simulated VIL Characteristics](image)

**Figure 6.3.2.4:** Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 140µs; Energy level of the shallow interface state = 0.4eV; Energy level of the deep interface state = 0.6eV.

**Observations and Analysis:**

1. The magnitude of the BTE luminance is large and it exhibits oscillations (Figure 6.3.2.4).
   
The BTE luminance persists even after the MTE luminance has begun.
   
The reason behind the presence of oscillations is described in Section 6.4.

2. The LE luminance exhibits a peak (Figure 6.3.2.4).

3. Many smaller luminance peaks are observed between the LE and BTE luminance peaks.
6.3.2.5: Depth of shallow interface state = 0.4eV; Depth of deep interface state = 0.7eV.

Figure 6.3.2.5: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 140µs; Energy level of the shallow interface state = 0.4eV; Energy level of the deep interface state = 0.7eV.

Observations and Analysis:

1. Conduction flux is clearly absent (Figure 6.3.2.5).
   
   a. Since the interface states are very deep, few electrons, if any, tunnel out of the interface. Hence, only displacement flux is seen in the VIL characteristics.

2. Luminance curve is clearly absent. This is because no electrons tunnel out into the phosphor bulk to cause any impact excitation or other luminance producing processes.
6.3.3. **Observations and Analysis:**

1. As the depth of the deepest interface state from the conduction band was increased, the displacement flux was more predominant than conduction flux. This is reasoned out as follows:
   a. A greater potential is necessary to eject the electrons from the deep cathodic interface states. Hence, when the interface states are much deeper, lesser number of electrons tunnel out into the phosphor and reach the other interface for the same applied potential than when the states are shallower.

2. The LE luminance was almost zero. This is reasoned out below:
   a. Since fewer electrons tunnel out of the cathodic interface, number of electrons colliding with the Cu atoms is less and hence, fewer excitations and relaxations take place within the Cu atoms. As a result, light emitted from the device is much less when the interface states are deeper (Figs. 6.3.2.3 and Figs. 6.3.2.4).

3. As the shallow and deep interface states are brought closer to each other, and their depths from the conduction band are decreased, more electrons are transferred to the other interface. This rapid transfer of electrons to the other interface results in a rapid build up of charges at the interfaces. This flow of electrons from one interface to another ionizes the activators present in the bulk and results in an increased space charge in the phosphor. As a result, a large internal electric field is set up in the phosphor, and the net field decreases. Hence, the flux tunneling out of the interface states also decreases after some time.

4. The leading edge luminance peak, attributed to impact excitation and subsequent relaxation (For details, refer Section 2.3 and Section 3.3), tracks the flux waveform very closely.

5. Thus, the shape of flux, and as a result, shape of luminance plots are also controlled by the depth of the interface states from the conduction band.
Section 6.4: Changing Threshold Electric Field for Dipole Collapse

6.4.1. Procedure:

Theoretical studies were performed to determine the effects of varying the threshold electric field at which dipoles collapse on the VIL characteristics of the ACTFEL device. The threshold electric field at which the dipoles collapsed in the phosphor was varied from 0.3MV/cm to 1.1MV/cm and simulations were performed. The resulting data was collected and VIL characteristics were plotted.
6.4.2. Results:

The VIL characteristics for different threshold fields for dipole collapse are plotted below:

6.4.2.1: Threshold Electric Field for Dipole Collapse = 0.3 MV/cm.

![Simulated VIL Characteristics with Threshold Electric Field for Dipole Collapse = 0.3 MV/cm](image)

Figure 6.4.2.1: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 0.3MV/cm.

Observations:

1. The BTE luminance exhibits multiple peaks (Figure 6.4.2.1). Oscillations are exhibited in these peaks.
6.4.2.2: Threshold Electric Field for Dipole Collapse = 0.4 MV/cm.

Figure 6.4.2.2: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 0.4MV/cm.

Observations:

1. The BTE luminance exhibits multiple peaks (Figure 6.4.2.2). Oscillations are exhibited in these peaks.
2. In addition to the multiple peaks, a number of smaller luminance peaks can be observed.
6.4.2.3: Threshold Electric Field for Dipole Collapse = 0.5 MV/cm.

**Figure**

6.4.2.3: *Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100μs; Threshold Field for Dipole Collapse = 0.5MV/cm.*

**Observations:**

1. The BTE luminance exhibits a single peak (Figure 6.4.2.3). Oscillations are observed in this peak.
2. In addition to the BTE luminance peak, a number of smaller luminance peaks spaced closer together are observed. These luminance peaks appear at the tail of the LE luminance and takes the form of a small shoulder.
6.4.2.4: Threshold Electric Field for Dipole Collapse = 0.6 MV/cm.

Figure 6.4.2.4: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 0.6MV/cm.

Observations:

1. The BTE luminance exhibits a single peak (Figure 6.4.2.4). Oscillations are observed in this peak.
2. In addition to the BTE luminance peak, a number of smaller luminance peaks are observed. Unlike being aggregated close together and near the LE luminance as in Figure 6.4.2.3, these peaks are spread out much wider and more evenly between the LE and BTE luminance peaks. These smaller peaks appear very close to the LE peak and manifests as a shoulder in the LE luminance.
6.4.2.5: Threshold Electric Field for Dipole Collapse = 0.7 MV/cm.

**Figure 6.4.2.5:** Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 0.7MV/cm.

**Observations:**

1. The BTE luminance exhibits a single peak (Figure 6.4.2.5). Oscillations are observed in this peak.

2. In addition to the BTE luminance peak, a number of smaller luminance peaks are observed. Unlike being aggregated close together and near the LE luminance as in Figure 6.4.2.3, these peaks are spread out much wider and more evenly in the luminance curve (Figure 6.4.2.5).
6.4.2.6: Threshold Electric Field for Dipole Collapse = 0.8 MV/cm.

Figure 6.4.2.6: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 0.8MV/cm

Observations:

1. The BTE luminance exhibits a single peak (Figure 6.4.2.6). Oscillations are observed in this peak.
2. In addition to the BTE luminance peak, a number of smaller luminance peaks are observed. Unlike being aggregated close together and near the LE luminance as in Figure 6.4.2.3, these peaks are spread out much wider and more evenly in the luminance curve (Figure 6.4.2.6). A small shoulder is visible in LE luminance.
6.4.2.7: Threshold Electric Field for Dipole Collapse = 0.9 MV/cm.

![Simulated VIL Characteristics with Threshold Electric Field for Dipole Collapse = 0.9 MV/cm](image)

**Figure**

6.4.2.7: *Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 0.9MV/cm.*

**Observations:**

1. The BTE luminance exhibits a single sharp peak (Figure 6.4.2.7).
2. In addition to the BTE luminance peak, a number of smaller luminance peaks are observed. These peaks occur much earlier than the main LE peak (Figure 6.4.2.7).
6.4.2.8: Threshold Electric Field for Dipole Collapse = 1.0 MV/cm.

Figure 6.4.2.8: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 1.0MV/cm.

Observations and Analysis:

1. The BTE luminance peak is clearly absent (Figure 6.4.2.9). This is because, dipoles have already collapsed before this time as evident from the numerous small peaks.

2. A number of small peaks are observed. These peaks begin to occur at around the same time instant as the main LE peak (Figure 6.4.2.9). It should, however, be noted that lesser number of such small peaks are present in the luminance plot for higher threshold fields than for lower threshold fields (Figs. 6.4.2.1 – 6.4.2.8).
6.4.2.9: Threshold Electric Field for Dipole Collapse = 1.1 MV/cm.

![Simulated VIL characteristics for driving voltage of 160V with Threshold Field for Dipole Collapse = 1.1 MV/cm](image)

**Figure 6.4.2.9:** Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Threshold Field for Dipole Collapse = 1.1 MV/cm.

**Observations:**

1. The BTE luminance peak is clearly absent (Figure 6.4.2.9).
2. A number of small peaks are observed. These peaks begin to occur at around the same time instant as the main LE peak (Figure 6.4.2.9). It should, however, be noted that lesser number of such small peaks are present in the luminance plot for higher threshold fields than for lower threshold fields (Figs. 6.4.2.1 – 6.4.2.7).
6.4.3. Observations and Analysis:

It was observed that varying the threshold electric field at which dipoles collapse had a significant impact on the BTE luminance (Figs. 6.4.2.1 to 6.4.2.9).

1. The peak value of BTE luminance increased as the threshold field for collapse of dipoles was increased until a particular threshold value and then the BTE peak was absent.

2. There were fewer oscillations in BTE luminance at higher threshold fields; at very high threshold fields, the oscillations were clearly absent and a single BTE luminance peak was observed.

3. The total area under the BTE luminance peak(s) was/were constant.

The observations are reasoned out below:

1. The BTE luminance is attributed to collapse of dipoles in the phosphor and subsequent relaxation of the electrons within the activators.

2. The time at which these dipoles collapse is determined by the time at which the net electric field in the phosphor goes below the threshold field.

3. The electric field varies both in time and space within the phosphor (Figure 6.6.1).

4. When the field in the phosphor goes below this threshold field, the dipoles in the sections where the net field is less than this threshold field, collapse. The dipoles in the other sections, however, do not collapse.

5. Because of spatial and temporal variation of electric field in phosphor, dipoles collapse at different times and in different sections in phosphor. Subsequent relaxation of the electrons within the activator produces light. Hence, the BTE peaks have a jagged waveform.

6. When the threshold field for dipole collapse is high, there are many sections within the phosphor where field is much below this threshold field (Figure 6.4.2.9). Hence, more dipoles collapse at nearly the same time instant resulting in a single large BTE peak.

7. When the threshold field is less, there are many sections in phosphor in which the field is much larger than the threshold field. The dipoles in these sections do not collapse until the field in these sections has fallen below the threshold field. Hence,
multiple, though smaller, peaks are seen for lesser threshold fields (Figs. 6.4.2.1 to 6.4.2.4).

8. The total number of dipoles present in the phosphor is, for practical purposes, constant. Hence, the total luminance produced as a result of their collapse and relaxation of the electron within the activator is also a constant. Hence, the area under the BTE luminance peak(s) is/are constant (Figs. 6.4.2.1 to 6.4.2.9).

9. The shoulder in the LE luminance was most predominant when simulations were performed setting the electric field at which the dipoles collapse within the range of 0.5 to 0.6 MV/cm (Figs. 6.4.2.3 and 6.4.2.4).
Section 6.5: Changing Number of Activators and Traps

6.5.1. Procedure:

The number of traps present in the phosphor was varied. Simulations were performed by setting the number of traps present in the activators to be less than the number of activators present. Subsequently, the number of traps present in the phosphor was increased to equal the number of activators. The simulated results are shown below:

6.5.2. Results:

6.5.2.1. Number of Traps = $10^{18}$ cm$^{-3}$

Figure 6.5.2.1: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Number of Traps = $10^{18}$ cm$^{-3}$.
Observations and Analysis:

1. The magnitude of BTE luminance is small (Figure 6.5.2.1).
   a. This is attributed to fewer dipoles being present in the bulk; this is a direct result of reducing the activator and trap density in the bulk.

2. A large MTE luminance peak is observed.

3. The LE luminance does not exhibit a peak.

4. Since fewer electrons are impact ionized from the Copper activators, the magnitude and rate of increase of internal electric field is much lesser than the magnitude and rate of increase of the applied electric field. Hence, flux and luminance curves do not exhibit well defined peaks and starts to decrease once the external field is constant.
6.5.2.2. **Number of Traps = \(5 \times 10^{18} \text{ cm}^{-3}\)**

**Observations and Analysis:**

1. The magnitude of the BTE luminance is large and it exhibits oscillations (Figure 6.5.2.2).
   a. Since large number of traps and activators are present in the device, more dipoles are formed. When, these dipoles collapse, more light is produced. The reason behind the presence of oscillations is described in Section 6.4.

2. The LE luminance exhibits a peak (Figure 6.5.2.2).
   a. A large number of electrons are impact ionized from the Copper activators, and hence, at some time instant (before the voltage reaches its maximum), the magnitude and rate of increase of internal electric field is greater than the magnitude and rate of increase of the applied electric field. At this time instant, the flux and luminance curves exhibit well defined peaks.
6.5.2.3. Number of Traps = $10^{19}$ cm$^{-3}$

**Figure**

6.5.2.3: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Number of Traps = $10^{19}$ cm$^{-3}$.

**Observations and Analysis:**

1. The magnitude of the BTE luminance is large and it exhibits oscillations (Figure 6.5.2.3).
2. The LE luminance exhibits a peak (Figure 6.5.2.3). These observations have been explained in Section 6.5.2.2.
3. Many smaller luminance peaks are observed between the LE and BTE luminance peaks. Since dipoles collapse at different times in different sections, such luminance peaks are observed. This has been explained in detail in Section 6.4 where the effect of varying the threshold field for dipole collapse on the BTE luminance has been presented.
6.5.2.4. Number of Traps = $2 \times 10^{19}$ cm$^{-3}$

**Figure**

*6.5.2.4: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100µs; Number of Traps = $2 \times 10^{19}$ cm$^{-3}$.*

**Observations and Analysis:**

1. The magnitude of the BTE luminance is large and it exhibits oscillations (Figure 6.5.2.4).

2. The LE luminance exhibits a peak (Figure 6.5.2.4).
   These observations have been explained in Section 6.5.2.2.

3. Many smaller luminance peaks are observed between the LE and BTE luminance peaks. Since dipoles collapse at different times in different sections, such luminance peaks are observed. This has been explained in detail in Section 6.4 where the effect of varying the threshold field for dipole collapse on the BTE luminance has been presented.
Chapter 7

CONCLUSION AND RECOMMENDATIONS FOR FUTURE WORK

7.1. Conclusion

An analytical model that described the optoelectronic processes occurring in the ACTFEL device was developed under the guidance of Dr. Singh and its validity was tested by means of numerical simulations. The numerical simulations qualitatively verify the accuracy of the model.

The device drive parameters were varied in order to study its effect on the VIL characteristics of the device. On varying the voltage applied to the device and its rise and fall times, a good insight was obtained into device behavior. Simulations were also performed to obtain responses to qualitatively match the experimentally obtained responses.

Various What-If scenarios have been studied by varying the parameters in the equations. These studies have indicated the importance of these parameters in determining device performance. These include, but are not limited to, threshold field for collapse of dipoles, densities at the interface states, depth of energy levels from the conduction band at the interface states, tunneling constants, rates of impact excitation and ionization and number of activators and traps.

7.2. Future Work

A quantitative match between the experimental and simulated characteristics needs to be achieved. In order to obtain such a fit, values of certain constants need to be modified. Efforts are currently underway to develop experimental techniques to obtain ranges of values that these constants can take. A detailed study of the interface states need to be performed as it was found to influence device behavior significantly.

A quantitative match will further establish the validity of the analytical model and will aid in developing more efficient blue ACTFEL devices.
APPENDIX A

SIMULATION CODE (PROG.C)

/************************************************************************
Title:  prog.c
Author: Praveen Sivakumar
************************************************************************/

#include <stdio.h>
#include <math.h>
#include "constants.h"  /* All the constants are defined here */
#include "variables.h"  /* All the global variables are declared here */

main() {
    void init();
    void exchange();
    void driver();
    void anodic_interface();
    void write_scaled_file();
    int k;
    Infofile = fopen("info.txt","w+" );
    Scaledfile1 = fopen("s_v","w+" );
    Scaledfile2 = fopen("s_f","w+" );
    Scaledfile3 = fopen("s_l","w+" );
    Timefile = fopen("time","w+" );
    Macrofile = fopen("all","w+" );
    VILfile = fopen("vil","w+" );
    E1file = fopen("e1","w+" );
    V = fopen ("v","w+" );
    LvsT = fopen("l", "w+" );
    CvsT[1] = fopen("ct1", "w+" );
    CvsT[5] = fopen("ct5", "w+" );
    CvsT[10] = fopen("e", "w+" );
    F1vsT = fopen("ft1", "w+" );
F5vsT = fopen("ft5", "w+" );
FnvsT = fopen("f", "w+" );
D1vsT = fopen("dt1", "w+" );
D5vsT = fopen("dt5", "w+" );
DnvsT = fopen("dtn", "w+" );
Ro1vsT = fopen("ro1", "w+" );
Ro5vsT = fopen("ro5", "w+" );
RonvsT = fopen("ron", "w+" );
NtvsT = fopen("t", "w+" );
RhovsT = fopen("s", "w+" );
R8vsT = fopen("temp", "w+" );
Ex500vsT = fopen("ex500", "w+" );
Rhox500vsT = fopen("rhox500", "w+" );
Ex1000vsT = fopen("ex1000", "w+" );
Rhox1000vsT = fopen("rhox1000", "w+" );
Ex2000vsT = fopen("ex2000", "w+" );
Rhox2000vsT = fopen("rhox2000", "w+" );
Ex3000vsT = fopen("ex3000", "w+" );
Rhox3000vsT = fopen("rhox3000", "w+" );
Ex4000vsT = fopen("ex4000", "w+" );
Rhox4000vsT = fopen("rhox4000", "w+" );
Ex4500vsT = fopen("ex4500", "w+" );
Rhox4500vsT = fopen("rhox4500", "w+" );
nahvsT = fopen("nah", "w+" );

flux_direction = 0;
init();
j = 1;
z = 1;

while( z <= NO_OF_PULSES)
{
    set_tunnel = 0;
fld_tunnel = 0;
t = 0;
printf("Pulse number %d is running currently \n", z);
if( z != 1)
    exchange();
driver();
anodic_interface();
write_scaled_file();
fprintf(Infofile,"Pulse Number: %d\n\n",z);
fprintf(Infofile,"Maximum Luminance = %f\n",max_lum);
fprintf(Infofile,"Maximum Flux = %f\n",max_flux);
fprintf(Infofile,"Maximum Cathodic Electric Field = %f\n",max_e_cathode);
fprintf(Infofile,"Maximum Anodic Electric Field = %f\n",max_e_anode);
fprintf(Infofile,"Total Luminance = %f\n\n\n",tot_luminance);
++z;
}
fclose(VILfile);
fclose(EIfile);
fclose(V);
fclose(LvsT);
fclose(CvsT[1]);
fclose(CvsT[5]);
fclose(CvsT[10]);
fclose(NSvsT);
fclose(D1vsT);
fclose(D5vsT);
fclose(DnvsT);
fclose(F1vsT);
fclose(F5vsT);
fclose(FnvsT);
fclose(Ro1vsT);
fclose(Ro5vsT);
fclose(RonvsT);
fclose(PatvsT);
fclose(PtcvsT);
fclose(NvsT);
fclose(R8vsT);
fclose(NtvsT);
fclose(Ex500vsT);
fclose(Ex1000vsT);
fclose(Ex2000vsT);
fclose(Ex3000vsT);
fclose(Ex4000vsT);
fclose(Ex4500vsT);
fclose(Rhox500vsT);
fclose(Rhox1000vsT);
fclose(Rhox2000vsT);
fclose(Rhox3000vsT);
fclose(Rhox4000vsT);
fclose(Rhox4500vsT);
fclose(Macrofile);
fclose(Scaledfile1);
fclose(Scaledfile2);
fclose(Scaledfile3);
fclose(Timefile);
fclose(nahvsT);
fclose(Infofile);
return;
}
void write_scaled_file(void)
{

max_lum = Lum[0];
tot_luminance = 0;
for(run_t = 0; run_t < t+1; run_t++)
{
    if (max_lum < Lum[run_t])
    {
        max_lum = Lum[run_t];
    }
    tot_luminance = tot_luminance + Lum[run_t];
}
max_e_cathode = e_cathode[0];
for(run_t = 0; run_t < t+1; run_t++)
{
    if (max_e_cathode < e_cathode[run_t])
    {
        max_e_cathode = e_cathode[run_t];
    }
}
for(run_t = 0; run_t < t+1; run_t++)
{
    e_cathode[run_t] = e_cathode[run_t] / max_e_cathode;
}
max_e_anode = e_anode[0];
for(run_t = 0; run_t < t+1; run_t++)
{
    if (max_e_anode < e_anode[run_t])
    {
        max_e_anode = e_anode[run_t];
    }
}
for(run_t = 0; run_t < t+1; run_t++)
\[
e_{anode}[run_t] = \frac{e_{anode}[run_t]}{max\_e\_anode};
\]
for (run_t = 0; run_t < t + 1; run_t++)
{
    Lum[run_t] = \frac{Lum[run_t]}{max\_lum};
}

max_v = Vol[0];
for (run_t = 0; run_t < t + 1; run_t++)
{
    if (max_v < Vol[run_t])
    {
        max_v = Vol[run_t];
    }
}
for (run_t = 0; run_t < t + 1; run_t++)
{
    Vol[run_t] = \frac{Vol[run_t]}{max_v};
}

max_flux = Flu[0];
for (run_t = 0; run_t < t + 1; run_t++)
{
    if (max_flux < Flu[run_t])
    {
        max_flux = Flu[run_t];
    }
}
for (run_t = 0; run_t < t + 1; run_t++)
{
    Flu[run_t] = \frac{Flu[run_t]}{max\_flux};
}
max_flux_disp = 0;
for(run_t = 1;run_t<t+1;run_t++)
{
    flux_disp = ((6.8624E-9)*((Vol[run_t]-Vol[run_t+1]))*max_v)/(q*delta_T);
    if (max_flux_disp < flux_disp)
    {
        max_flux_disp = flux_disp;
    }
}
max_flux_disp = max_flux_disp/max_flux;
if (z==199)
{
    for (run_t=1;run_t<(t+1001);run_t++)
    {
        flux_disp = ((6.8624E-9)*((Vol[run_t]-Vol[run_t+1]))*max_v)/(q*delta_T);
        if ((z % 2)!= 0)
        {
            if (run_t < flux_point)
            {
                tot_flux_unscaled = Flu[run_t]+(flux_disp/max_flux);
                tot_flux_scaled = tot_flux_unscaled/(1+max_flux_disp);
                fprintf(Scaledfile1,"%.5lf \n",Vol[run_t-1]);
                fprintf(Scaledfile2,"%.5lf \n",Lum[run_t]);
                fprintf(Scaledfile3,"%.5lf \n",tot_flux_scaled);
                fprintf(Timefile,"%f \n",(run_t)*delta_T);
            }
            if (run_t > flux_point)
            {
                tot_flux_unscaled = -Flu[run_t]+(flux_disp/max_flux);
                tot_flux_scaled = tot_flux_unscaled/(1+max_flux_disp);
            }
        }
    }
}
fprintf(Scaledfile1,"%.5lf\n",Vol[run_t-1]);
fprintf(Scaledfile2,"%.5lf\n",Lum[run_t]);
fprintf(Scaledfile3,"%.5lf\n",tot_flux_scaled);
fprintf(Timefile,"%f \n",(run_t)*delta_T);
}
}
else
{
if (run_t < flux_point)
{
    tot_flux_unscaled = Flu[run_t]+(flux_disp/max_flux);
tot_flux_scaled = tot_flux_unscaled/(1+max_flux_disp);
fprintf(Scaledfile1,"%.5lf\n",-Vol[run_t-1]);
fprintf(Scaledfile2,"%.5lf\n",Lum[run_t]);
fprintf(Scaledfile3,"%.5lf\n",-tot_flux_scaled);
fprintf(Timefile,"%f \n",(run_t)*delta_T);
}
if (run_t > flux_point)
{
    tot_flux_unscaled = -Flu[run_t]+(flux_disp/max_flux);
tot_flux_scaled = tot_flux_unscaled/(1+max_flux_disp);
fprintf(Scaledfile1,"%.5lf\n",-Vol[run_t-1]);
fprintf(Scaledfile2,"%.5lf\n",Lum[run_t]);
fprintf(Scaledfile3,"%.5lf\n",-tot_flux_scaled);
fprintf(Timefile,"%f \n",(run_t)*delta_T);
}
}
}

void driver ( void ){
int k ;  
int Ts1; 
void constants();  
void cathodic_tunneling();  
void bulk_phosphor();  
void shallow_states();  
Vapp = 0;  
for(i=1;i<=(2*Ts);++i)  
   {  
      ctr_i = i;  
      if( i <= RISE_TIME )  
      {  
         Vapp += (Vs/RISE_TIME);  
      }  
      if((i>RISE_TIME) && (i<=FALL_TIME))  
      {  
         Vapp=Vs;  
      }  
      if( (i > FALL_TIME) && (i <= Ts) ) {  
         Vapp -= (Vs/(Ts-FALL_TIME));  
      }  
      constants();  
      cathodic_tunneling();  
      bulk_phosphor();  
      if (z==199)  
      {  
         if ((z % 2)!= 0)  
         {  
            fprintf(V,"%f       %4.3lf \n",ctr_i*delta_T*1E6,Vapp);  
            fprintf(D1vsT, "%f        %.5lf \n", ctr_i*delta_T*1E6,Nao-nal[1]-nah[1] );  
            fprintf(D5vsT, "%f        %.5lf \n", ctr_i*delta_T*1E6,Nao-nal[5]-nah[5] );  
            fprintf(DnvsT, "%f        %.5lf \n", ctr_i*delta_T*1E6,Nao-nal[n]-nah[n] );  
         }  
      }  
}
fprintf(Ro1vsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[1]-nah[1]-nt2[1]);
fprintf(Ro5vsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[5]-nah[5]-nt2[5]);
fprintf(RonvsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[n]-nah[n]-nt2[n]);
if (flux_direction == 0)
{
    if (i<=RISE_TIME)
    {
        fprintf(F1vsT, "%.5lf 
", ctr_i*delta_T*1E6,Fn[1]);
        fprintf(F5vsT, "%.5lf 
", ctr_i*delta_T*1E6,Fn[2]);
        fprintf(FnvsT, "%.5lf 
", ctr_i*delta_T*1E6,Fn[n]+fluxDisp);
        fprintf(Macrofile,"%.5lf %.51f %.51f %.51f
",ctr_i*delta_T*1E6,Vapp,(Fn[n]+fluxDisp)*6.25E-16,Lt*1E3);
    }
    if ((i>=(Ts-FALL_TIME))&&(i<=FALL_TIME))
    {
        fprintf(F1vsT, "%.5lf 
", ctr_i*delta_T*1E6,Fn[1]);
        fprintf(F5vsT, "%.5lf 
", ctr_i*delta_T*1E6,Fn[2]);
        fprintf(FnvsT, "%.5lf 
", ctr_i*delta_T*1E6,Fn[n]-fluxDisp);
        fprintf(Macrofile,"%.5lf %.51f %.51f %.51f
",ctr_i*delta_T*1E6,Vapp,(Fn[n]-fluxDisp)*6.25E-16,Lt*1E3);
    }
}
if (flux_direction == 1)
{
    if (i<=RISE_TIME)
    {
        fprintf(F1vsT, "%.5lf 
", ctr_i*delta_T*1E6,-Fn[1]);
        fprintf(F5vsT, "%.5lf 
", ctr_i*delta_T*1E6,-Fn[2]);
        fprintf(FnvsT, "%.5lf 
", ctr_i*delta_T*1E6,-Fn[n]+fluxDisp);
        fprintf(Macrofile,"%.5lf %.51f %.51f %.51f
",ctr_i*delta_T*1E6,Vapp,(-Fn[n]+fluxDisp)*6.25E-16,Lt*1E3);
    }
}
if ((i>=(Ts-FALL_TIME))&&(i<=FALL_TIME))
{
    fprintf(F1vsT, "%.5lf \n", ctr_i*delta_T*1E6,-Fn[1]);
    fprintf(F5vsT, "%.5lf \n", ctr_i*delta_T*1E6,-Fn[2]);
    fprintf(FnvsT, "%.5lf \n", ctr_i*delta_T*1E6,-Fn[n]-flux_disp);
    fprintf(Macrofile,"%.5lf %51f %51f %51f \n",ctr_i*delta_T*1E6,Vapp,(-Fn[n]-flux_disp)*6.25E-16,Lt*1E3);
}
}
fprintf(NtvsT, "%.5lf \n", ctr_i*delta_T*1E6,nt2[n]);
fprintf(R8vsT, "%.5lf-%5lf\n", ctr_i*delta_T*1E6,total_charge,(R3[n] + R13[n] - R9[n]));
}
else
{
    fprintf(V,"%.4f \n",ctr_i*delta_T*1E6,-(Vapp));
    fprintf(D1vsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[1]-nah[1] );
    fprintf(D5vsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[5]-nah[5] );
    fprintf(DnvsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[n]-nah[n] );
    fprintf(Ro1vsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[1]-nah[1]-nt2[1] );
    fprintf(Ro5vsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[5]-nah[5]-nt2[5] );
    fprintf(RonvsT, "%.5lf\n", ctr_i*delta_T*1E6,Nao-nal[n]-nah[n]-nt2[n] );
    if (flux_direction == 0)
    {
        if (i<=RISE_TIME)
        {
            fprintf(F1vsT, "%.5lf \n", ctr_i*delta_T*1E6,-Fn[1]);
            fprintf(F5vsT, "%.5lf \n", ctr_i*delta_T*1E6,-Fn[2]);
            fprintf(FnvsT, "%.5lf \n", ctr_i*delta_T*1E6,-Fn[n]+flux_disp);
fprintf(Macrofile,"%f %.5lf %.5lf %.5lf\n",ctr_i*delta_T*1E6,Vapp,(-Fn[n]+flux_disp)*6.25E-16,Lt*1E3);
}
if ((i>=(Ts-FALL_TIME))&&(i<=FALL_TIME))
{
fprintf(F1vsT, "%f %.5lf \n", ctr_i*delta_T*1E6,-Fn[1]);
fprintf(F5vsT, "%f %.5lf \n", ctr_i*delta_T*1E6,-Fn[2]);
fprintf(FnvsT, "%f %.5lf \n", ctr_i*delta_T*1E6,-Fn[n]-flux_disp);
fprintf(Macrofile,"%f %.5lf %.5lf %.5lf\n",ctr_i*delta_T*1E6,Vapp,(-Fn[n]-flux_disp)*6.25E-16,Lt*1E3);
}
}
if (flux_direction == 1)
{
if (i<=RISE_TIME)
{
fprintf(F1vsT, "%f %.5lf \n", ctr_i*delta_T*1E6,Fn[1]);
fprintf(F5vsT, "%f %.5lf \n", ctr_i*delta_T*1E6,Fn[2]);
fprintf(FnvsT, "%f %.5lf \n", ctr_i*delta_T*1E6,Fn[n]+flux_disp);
fprintf(Macrofile,"%f %.5lf %.5lf %.5lf\n",ctr_i*delta_T*1E6,Vapp,(Fn[n]+flux_disp)*6.25E-16,Lt*1E3);
}
if ((i>=(Ts-FALL_TIME))&&(i<=FALL_TIME))
{
fprintf(F1vsT, "%f %.5lf \n", ctr_i*delta_T*1E6,Fn[1]);
fprintf(F5vsT, "%f %.5lf \n", ctr_i*delta_T*1E6,Fn[2]);
fprintf(FnvsT, "%f %.5lf \n", ctr_i*delta_T*1E6,Fn[n]-flux_disp);
fprintf(Macrofile,"%f %.5lf %.5lf %.5lf\n",ctr_i*delta_T*1E6,Vapp,(Fn[n]-flux_disp)*6.25E-16,Lt*1E3);
}
}
fprintf(NtvsT, "%f \n ", ctr_i*delta_T*1E6,nt2[n]);
fprintf(R8vsT, "%f \%.51f \%.51f\n", ctr_i*delta_T*1E6,total_charge,(R3[n] + R13[n] - R9[n]));
}
Lt = 0;
nahct = 0;
for(k = 1; k <= n; ++k) {
    Lt += (Lit[k]);
    nahct = nahct + nah[k];
    if (i==1000) {
        fprintf(Ex500vsT, "%.51f \n ", c3[k]);
        fprintf(Rhox500vsT, "%.51f \n ", Nao-nal[k]-nah[k]);
    }
    if (i==2000) {
        fprintf(Ex1000vsT, "%.51f \n ", c3[k]);
        fprintf(Rhox1000vsT, "%.51f \n ", Nao-nal[k]-nah[k]);
    }
    if (i==4500) {
        fprintf(Ex2000vsT, "%.51f \n ", c3[k]);
        fprintf(Rhox2000vsT, "%.51f \n ", Nao-nal[k]-nah[k]);
    }
    if (i==7000) {
        fprintf(Ex3000vsT, "%.51f \n ", c3[k]);
        fprintf(Rhox3000vsT, "%.51f \n ", Nao-nal[k]-nah[k]);
    }
    if (i==8000) {
        fprintf(Ex4000vsT, "%.51f \n ", c3[k]);
fprintf(Rhox4000vsT, "%.51f\n", Nao-nal[k]-nah[k]);

if (i==9000) {
    fprintf(Ex4500vsT, "%.51f\n", c3[k]);
    fprintf(Rhox4500vsT, "%.51f\n", Nao-nal[k]-nah[k]);
}

} tot_lit = B * nahct * (Wz/TAU2);
e_cathode[t] = c3[1];
e_anode[t] = c3[n];
Lum[t] = tot_lit;
Vol[t] = Vapp;
Flu[t] = Fn[n];
t++;
fprintf(LvsT, "%f %.35lf\n", ctr_i*delta_T*1E6,Lt);
fprintf(nahvsT, "%.35lf\n",nahct);
fprintf(VILfile, "%f %.5lf %.5lf %.5lf\n", 
ctr_i*delta_T*1E6,Vapp*1E4,Fn[n]*1E-06,Lt*0.7E14);
fprintf(EIfile,"%f %.51f %.51f\n",ctr_i*delta_T*1E6,c3[n],Fn[n]*1E-06);
}
++j;
}
return;
}

void init (void)
{
    int k;
    for ( k=1; k<=n; ++k )
    {

nah[k] = 0;
nt2[k] = 0;
na1[k] = Nao-nt2[k];
Fn[k] = 0;
condnband[k] = 0;
}
Fn[0]= 0;
nc1 = 0.0*Neq;
nc11 = Neq;
a1 = 0.0*Neq;
a11 = Neq;
flux_dis = 0.6863E17;
return;
void cathodic_tunneling(void)
{
    double fld,nc1r,nc2r,nc3r,nc4r,nc5r,nc6r,nc7r,nc8r,nc9r,nc10r,nc11r;
    double Pc1,Pc11,d1,d11;
    double f1,f11;
    fld = c3[1];
    if(fld<0)
    {
        Fn[0]=0;
    }
    else
    {
        d1 = (-b1) * pow( ( m/m_star), -0.5) * pow(E1, 1.5) * (1/fld);
        d11 = (-b1) * pow( ( m/m_star), -0.5) * pow(E11,1.5)  * (1/fld);
        Pc1 = a1 * pow( ( m/m_star), 0.125) * pow( E1, 0.625) * pow(fld, 0.25) * exp(d1);
        Pc11= a1 * pow( ( m/m_star), 0.125) * pow( E11, 0.625) * pow(fld,0.25) * exp(d11);
        f1 = nc1*Pc1;
    }
}
f11 = nc11*Pc11;
if(f1>nc1/delta_T)
{
    f1 = nc1/delta_T;
}
if(f11>nc11/delta_T)
{
    f11 = nc11/delta_T;
}
if(f1<0)
{
    printf("f1<0 => Error in cathodic interface \n");
    exit();
}
if(f11<0)
{
    printf("f11<0 => Error in cathodic interface \n");
    exit();
}
nc1 = nc1 - (f1 * delta_T);
if (nc1<0)
{
    f1 = f1+nc1/delta_T;
    nc1 = 0;
}
nc11 = nc11 - (f11*delta_T);
if (nc11<0)
{
    f1 = f1+nc11/delta_T;
    nc11 = 0;


```c
Fn[0] = f1 + f11;
if (set_tunnel==0)
{
    if ((f1+f11)>1E16)
    {
        fld_tunnel = c3[1];
        set_tunnel = 1;
    }
}
return;
}
void bulk_phosphor(void)
{
    int k;
    double fld;
    double fldc;
    double flda;
    double d1, d2;
    double dnal, dnaht, dnt2dt, dnah;
    double d1dt, d11dt, d1_11dt;
    double PEALE1;
    void cathodic_interface();
    void anodic_interface();
    void anodic_tunneling();
    fldc = c3[1];
    flda = c3[n];
    Fn[n] = 0;
    total_charge = nc1+nc11+na1+na11;
    if (flda < 0)
```
anodic_tunneling();

if (Fn[0]>Fn[n])
{
    for (k=1;k<=n;k++)
    {
        fld = c3[k];
        fnew1 = 0;
        fnew2 = 0;
        fprimenew2 = 0;
        if (fld<0)
        {
            fld = -fld;
        }
        if (fld<(0.3E6))
        {
            fnew1 = 0;
            fnew2 = 0;
            fprimenew2 = 0;
        }
        if ((fld>(0.3E6))&&(fld<(0.65E6)))
        {
            fnew1 = ((fld-(0.3E6))/(0.35E6))*((fld-(0.3E6))/(0.35E6));
            fnew2 = 0;
            fprimenew2 = 0;
        }
        if ((fld>(0.65E6))&&(fld<(1.1E6)))
        {
            fnew2 = 0.33*(((fld-(0.65E6))/(0.45E6))*(((fld-(0.65E6))/(0.45E6)));
        }
    }
}

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fprimenew2 = 0.67*(((fld-(0.65E6)))/(0.45E6))*(((fld-(0.65E6)))/(0.45E6));

fnew1 = 1 - (fnew2+fprimenew2);

}  
if (fld>(1.1E6))
{
  fnew2 = 0.33;
  fprimenew2 = 0.67;
  fnew1 = 0;
}

Lit[k] = B * nah[k] * (Wx/TAU2) ;
actcharge[k] = Nao-nal[k]-nah[k];
Prob = nal[k]*3.14*radius*radius;
Prob2 = nah[k]*3.14*radius*radius;
R1[k] = (Fn[k-1])*fnew1*Prob;
R4[k] = nah[k]/TAU2;
if (nt2[k] > Nt2)
{
  nt2[k] = Nt2;
}
pt = Nt2-nt2[k];
if (nal[k] <= pt)
{
  R2A[k] = (Fn[k-1])*fnew2*fnew3*Prob;
}
if (nal[k] > pt)
{
  R2A[k] = pt*(Fn[k-1])*fnew2*fnew3*3.14*radius*radius;
}
R2[k] = R2A[k];
if (nah[k] <= pt)
\[
\{ \\
\quad R_{12A}[k] = (F_n[k-1])f_{primenew2}\cdot f_{primenew3}\cdot Prob2; \\
\}
\]
if (nah[k] > pt)
\{
\quad R_{12A}[k] = pt*(F_n[k-1])f_{primenew2}\cdot f_{primenew3}\cdot 3.14\cdot r_{\text{adi}}\cdot r_{\text{adi}};
\}
R_{12}[k] = R_{12A}[k];
R_{8}[k] = 0;
if (fld > 600000)
\{
\quad \sigma_8 = 0;
\}
if (fld \leq 600000)
\{
\quad \sigma_8 = 1;
\}
if (n_{t2}[k] \leq (N_{ao} - n_{al}[k] - n_{ah}[k] - c_{ondnband}[k]))
\{
\quad R_{8}[k] = n_{t2}[k]\cdot \sigma_8/(\delta_{T_{dipole}});
\}
if (n_{t2}[k] > (N_{ao} - n_{al}[k] - n_{ah}[k] - c_{ondnband}[k]))
\{
\quad R_{8}[k] = (N_{ao} - n_{al}[k] - n_{ah}[k] - c_{ondnband}[k])\cdot \sigma_8/(\delta_{T_{dipole}});
\}
R_{3}[k] = (F_n[k-1])f_{new2}\cdot (1 - f_{new3}) \cdot \text{Prob};
R_{13}[k] = (F_n[k-1])f_{primenew2}(1-f_{primenew3})\cdot \text{Prob2};
R_{5}[k] = 0;
R_{9}[k] = 0;
d_{\text{nal}}dt = R_{4}[k] - R_{1}[k] - R_{2}[k] - R_{3}[k];
dnahdt = R1[k] - R4[k] + R8[k] - R12[k] + R9[k] - R13[k] + R5[k];
dnt2dt = R12[k] - R8[k] + R2[k];
Fn[k] = Fn[k-1] + (R3[k] + R13[k] - R9[k])*Wx;
dnt2 = dnt2dt * delta_T;
nt2[k] += dnt2;
dnal = dnaldt * delta_T;
nal[k] += dnal;
dnah = dnahdt * delta_T;
nah[k] += dnah;
condnband[k] = (R3[k] + R13[k] - R9[k])*delta_T;
total_charge = total_charge+(Nao-(nal[k]+nah[k]+nt2[k]))*Wx;
}
flux_direction = 0;
anodic_interface();
}
else
{
    Fn[n+1] = Fn[n];
    for (k=n;k>=1;k--)
    {
        fld = c3[k];
        fnew1 = 0;
        fnew2 = 0;
        fprimenew2 = 0;
        if (fld<0)
        {
            fld = -fld;
        }
        if (fld<(0.3E6))
        {
            fnew1 = 0;
        }
}
fnew2 = 0;
fprimenew2 = 0;
}
if ((fld>(0.3E6))&&(fld<(0.65E6)))
{
    fnew1 = ((fld-(0.3E6))/(0.35E6))*((fld-(0.3E6))/(0.35E6));
    fnew2 = 0;
    fprimenew2 = 0;
}
if ((fld>(0.65E6))&&(fld<(1.1E6)))
{
    fnew2 = 0.33*(((fld-(0.65E6)))/(0.45E6))*(((fld-(0.65E6)))/(0.45E6));
    fprimenew2 = 0.67*(((fld-(0.65E6)))/(0.45E6))*(((fld-(0.65E6)))/(0.45E6));
    fnew1 = 1 - (fnew2+fprimenew2);
}
if (fld>(1.1E6))
{
    fnew2 = 0.33;
    fprimenew2 = 0.67;
    fnew1 = 0;
}
Lit[k] = B * nah[k] * (Wx/TAU2) ;
actcharge[k] = Nao-nal[k]-nah[k];
Prob = nal[k]*3.14*radiu*radiu;
Prob2 = nah[k]*3.14*radiu*radiu;
R1[k] = (Fn[k+1])*fnew1*Prob;
R4[k] = nah[k]/TAU2;
if (nt2[k] > Nt2)
{
    nt2[k] = Nt2;
pt = Nt2-nt2[k];
if (nal[k] <= pt)
{
    R2A[k] = (Fn[k+1])*fnew2*fnew3*Prob;
}
if (nal[k] > pt)
{
    R2A[k] = pt*(Fn[k+1])*fnew2*fnew3*3.14*radiu*radiu;
}
R2[k] = R2A[k];
if (nah[k] <= pt)
{
    R12A[k] = (Fn[k+1])*fprimenew2*fprimenew3*Prob2;
}
if (nah[k] > pt)
{
    R12A[k] = pt*(Fn[k+1])*fprimenew2*fprimenew3*3.14*radiu*radiu;
}
R12[k] = R12A[k];
R8[k] = 0;
if (fld > 600000)
{
    sigma8=0;
}
if (fld <= 600000)
{
    sigma8=1;
}
if (nt2[k] <= (Nao-nal[k]-nah[k]-condnband[k]))
{

R8[k] = nt2[k]*sigma8/(delta_Tdipole);
}
if (nt2[k] > (Nao-nal[k]-nah[k]-condnband[k]))
{
    R8[k] = (Nao-nal[k]-nah[k]-
    condnband[k])*sigma8/(delta_Tdipole);
}
R3[k] = (Fn[k+1])*fnew2*(1 - fnew3) * Prob;
R13[k] = (Fn[k+1])*fprimenew2*(1-fprimenew3)*Prob2;
R9[k] = 0;
if ((Fn[k+1]/Wx) > actcharge[k]/delta_T)
{
    R5[k] = (actcharge[k])/delta_T;
}
else
{
    R5[k] = Fn[k+1]/Wx;
}
dnaldt = R4[k] - R1[k] - R2[k] - R3[k];
dnahdt = R1[k] - R4[k] + R8[k] - R12[k] + R9[k] - R13[k] + R5[k];
dnt2dt = R12[k] - R8[k] + R2[k];
Fn[k] = Fn[k+1] + (R3[k] +R13[k] - R9[k])*Wx;
dnt2 = dnt2dt * delta_T;
nt2[k] += dnt2;
dnal = dnaldt * delta_T;
nal[k] += dnal;
dnah = dnahdt * delta_T;
nah[k] += dnah;
condnband[k] = (R3[k] + R13[k] - R9[k] - R5[k])*delta_T;
total_charge = total_charge+(Nao-(nal[k]+nah[k]+nt2[k]))*Wx;
if (flux_direction == 0)
{
    flux_point = i;
}
flux_direction = 1;
cathodic_interface();
}
return;
}
void anodic_tunneling(void)
{
    double fld1;
    double Pa1,Pa11,d1,d11;
    double f1,f11;
    fld1 = c3[n];
    if(fld1>0)
    {
        Fn[n]=0;
    }
    else
    {
        fld1 = -fld1;
    }

d1 = (-b2) * pow( ( m/m_star), -0.5) * pow(E1, 1.5) * (1/fld1);
d11 = (-b2) * pow( ( m/m_star), -0.5) * pow(E11,1.5) * (1/fld1);
Pa1 = a2 * pow( ( m/m_star), 0.125) * pow( E1, 0.625) * pow(fld1, 0.25) * exp(d1);
Pa11= a2 * pow( ( m/m_star), 0.125) * pow( E11, 0.625) * pow(fld1,0.25) * exp(d11);
f1 = na1*Pa1;
f11 = na11*Pa11;
if(f1>na1/delta_T)
    {
f1=na1/delta_T;
}

if(f11>na11/delta_T)
{
    f11=na11/delta_T;
}

if(f1<0)
{
    printf("f1<0 => Error in anodic interface \n");
    exit();
}

if(f11<0)
{
    printf("f11<0 => Error in anodic interface \n");
    exit();
}

Fn[n] = f1 + f11;
na1 = na1 - (f1*delta_T);
if (na1<0)
{
    f1 = f1+na1/delta_T;
    na1 = 0;
}

na11 = na11 - (f11*delta_T);
if (na11<0)
{
    f11 = f11+na11/delta_T;
    na11 = 0;
}

return;
```c
void cathodic_interface()
{
    double dn1dt, dn11dt, dn1_11dt;
    dn1_11dt = nc1*Snd*Vth*(N11-nc11);
    dn1dt = Fn[1]-dn1_11dt;
    dn11dt = dn1_11dt;
    nc1 = nc1 + (dn1dt*delta_T);
    if (nc1<0)
    {
        nc1 = nc1-(dn1dt*delta_T);
        nc1 = nc1+(Fn[1]*delta_T);
    }
    else
    {
        nc11 = nc11 + (dn11dt*delta_T);
    }
}

void anodic_interface()
{
    double dn1dt, dn11dt, dn1_11dt;
    if (Fn[n] <0)
    {
        Fn[n] = - Fn[n];
    }
    dn1_11dt = na1*Snd*Vth*(N11-na11);
    dn1dt = Fn[n]-dn1_11dt;
    dn11dt = dn1_11dt;
    na1 = na1 + (dn1dt*delta_T);
    if (na1<0)
    {
```
void exchange(void) {
    int k;
    double temp1, temp2, temp3, temp4, temp5, temp6, temp7, temp8, temp9, temp10, temp11;
    for (k = 0; k < n/2; ++k) {
        nal[k+1] = nal[n-k];
        nah[k+1] = nah[n-k];
        nt2[k+1] = nt2[n-k];
        Fn[k+1] = Fn[n-k] = 0;
    }
    Fn[0] = 0;
    temp1 = nc1;
    nc1 = na1;
    na1 = temp1;
    temp11 = nc11;
    nc11 = na11;
    na11 = temp11;
    return;
}

void constants(void) {
    int k, t;
    double A1, A2, A3, A4, A5, A6, A7;
    double sum, sum1, sum2;
for( k=1; k<=n; ++k )
{
    activatorcharge[k]=Nao-nal[k]-nah[k];
    spacecharge[k]=activatorcharge[k]- nt2[k];
}

sum = 0;
for( k=1; k<=n-1; ++k)
    sum += spacecharge[k];

A7 = 2*W1 + ( ((n*Wx*ed)/ez) );
A1 = (q*W1*(na1+na2+na3+na4+na5+na6+na7+na8+na9+na10+na11-Neq))/ed;
A2 = ((W1*ez/ed) + n*Wx) * (q/ez) *
(nc1+nc2+nc3+nc4+nc5+nc6+nc7+nc8+nc9+nc10+nc11-Neq) ;
A3 = (q*Wx*W1*spacecharge[n])/ed;
A4 = ( (q*Wx*Wx)/(2*ez) ) * (sum + spacecharge[n]) ;
A5 = ( (q*Wx)/ez ) * ( Wx + ((W1*ez)/ed) ) * sum ;

sum1 = 0;
for( t=2; t<=(n-1); ++t) {
    sum2 = 0;
    for(k=1; k<=(t-1); ++k)
        sum2 += spacecharge[k];
    sum1 += sum2;
}

A6 = (q*Wx*Wx) * sum1 * (1/(ez));
c1 = ( Vapp + A1 + A2 - A3 - A4 - A5 - A6 ) / A7 ;
c3[1] = ( (ed * c1) - ( q * ( nc1 + nc2 + nc3+nc4+nc5+nc6+nc7+nc8+nc9+nc10+nc11 - Neq ) ) ) / ez;
for(k=1; k<=n-1; ++k) {
    c3[k+1] = c3[k] + ((q*spacecharge[k]*Wx)/ez) ;
}

if ((z==199)|((z==200))
{
    if (z % 2 !=0)
{  
  fprintf(CvsT[10], "%.5lf\n", i*delta_T*1E6,c3[n] );  
  fprintf(CvsT[5], "%.5lf\n", i*delta_T*1E6,c3[5] );  
  fprintf(CvsT[1], "%.5lf\n", i*delta_T*1E6,c3[1] );
}
else
{
  fprintf(CvsT[10], "%.5lf\n", i*delta_T*1E6,-(c3[n]) );  
  fprintf(CvsT[5], "%.5lf\n", i*delta_T*1E6,-(c3[5]) );  
  fprintf(CvsT[1], "%.5lf\n", i*delta_T*1E6,-(c3[1]) );
}
}
c5 = ( (ez*c3[n]) + (q * spacecharge[n] * Wx) - (q *
(na1+na2+na3+na4+na5+na6+na7+na8+na9+na10+na11-Neq)) ) / ed ;  
return;
}
APPENDIX B

HEADER FILE DECLARING CONSTANTS (CONSTANTS.H)

/* All the constants are defined here for actfel.c */
#define fnew1 0.05
#define delta1 1.0E-15
#define radiu 10.0E-8
#define fnew2 0.01
#define fnew4 0.005
#define beta1 1.0E-17
#define beta2 1.0E-6
#define fnew3 0.63
#define fprimenew2 0.02
#define G1 1.0E-14
#define tau1 1.75E-6
#define beta1p 2.53E-13
#define beta2p 2.53E-2
#define f2p 0.2
#define sigma5 0.4E-3
#define mobility 100
#define sigma9 1
#define delta_Tdipole 0.05E-06
#define E11 3
#define delta_T 0.05E-06
#define Ts 4500 /*Pulse-width*/ /*Pulse Width in terms of 50 nanoseconds*/
   /*slices can be set by the user */
#define Vs 160.0 /* Amplitude of the applied voltage */
#define RISE_TIME 1000 /*# of time slices of 50ns reqd. for the applied*/
   /* Voltage to rise from 0 to the peak voltage */
#define FALL_TIME 3500 /*# of time slices of 50ns. duration reqd. */
   /* for applied voltage to fall from peak to 0 */
#define NO_OF_PULSES 1 /* Number of pulses for which the program*/
/* should run */

#define Nt2 1.0E17 /*Density of states at trap level Et2 */
#define Nao 1.0E19 /*Equilibrium conc. of activators */
#define Nc 3.14E+18 /*Density of states in condn.band of phosphor.*/
#define N1 5.0E+13 /*Density of first interface states*/
#define N2 5.5E+13
#define N3 6.0E+13
#define N4 6.5E+13
#define N5 7.0E+13
#define N6 7.5E+13
#define N7 8.0E+13
#define N8 8.5E+13
#define N9 9.0E+13
#define N10 9.5E+13
#define N11 10.0E+13
#define SIGMA2 1.0E-8 /*This is the efficiency of electron */
/* transfer from activators to empty bulk traps*/
#define SIGMA1 5.0E-11 /*Effective electron capture coefficient*/
/*of level Eah from Et2 */
#define SIGMA3 4.0E-5 /*Effective electron capture coefficient */
/*of level Eah from Eis */
#define Sn 1.0E-17 /*Capture cross section area for thermal excitation*/
/* of electrons from Et2 to Ec. */
#define Snt 1.0E-16 /* Capture CS area for recomb. of electrons*/
/* from Ec to Et2 */
#define Vth 2.33E+07 /* Thermal Velocity of electrons */
#define Vsat 1.0E+07 /*saturation velocity of electrons in phosphor*/
#define Eb 1.06 /*Effective energy barrier to field assisted */
/* tunneling from Eal to Et2 */
#define Etc 0.58 /*Energy barrier to electron transfer from Et2 to Ec*/
#define KT 0.0259
# define a1  9.0E+10
# define b1 1.49E+08  /* a1 and b1 are constants */
# define m 9.1E-31    /* mass of an electron */
# define m_star 2.28E-31 /*Effective mass of an electron */
# define ALPHA 2.0E-16 /*Capture CSarea for impact excitation of activators*/
# define TAU2  0.05E-06 /*Time const for relaxation from Eah to Eal */
# define Neq  5.0E+13   /*Density of electrons at interface states at equilibrium*/
# define Nto 0         /*Density of bulk trap levels at Et(cm**3) */
#define E1 0.40                 /*Depth of energy level of first state from cond.band */
#define E2 0.41
#define E3 0.42
#define E4 0.43
#define E5 0.44
#define E6 0.45
#define E7 0.46
#define E8 0.47
#define E9 0.48
#define E10 0.49
#define E11 0.50 /*Depth of deeper level from cond.band at cathodic interface*/
#define q -1.6E-19 /* + or -  electronic charge*/
#define ez 83.19E-14 /*dielectric constant of phosphor */
#define ed 69.92E-14 /*dielectric constant of insulator layers */
//# define ed 187E-14 /*dielectric constant of insulator layers */
#define n 10       /* Number of sections */
#define Wz 0.67E-4 /*Width of phosphor layer */
#define Wx 0.67E-5 /*Width of each section of phosphor*/
#define B 3.9E-19 /*Light output for single transition from Eah to Eal*/
#define Snd 2.2E-17 /*capture CSarea for relaxation of electrons from Eis to Eid*/
#define W1 2.3E-5 /*Thickness of each insulator layer*/
APPENDIX C

HEADER FILE DECLARING VARIABLES (VARIABLES.H)

/* All the global variables are declared here for the program r.c*/

FILE *LvsT,*CvsT[n+1],*PatvsT,*PtcvsT,*D1vsT,*D5vsT,*DnvsT,*FvsT, *DvsT, *RhovsT,
*DvsT,*F1vsT,*F5vsT,*FnvsT,*NtvsT,*NvsT, *V, *NSvsT, *Ro1vsT, *Ro5vsT, *RonvsT,
/*These are all file-pointers*/
double R1[n+1],R2[n+1],R3[n+1],R4[n+1],R5[n+1],R6[n+1], R7[n+1], R8[n+1], R9[n+1],
R10[n+1], R11[n+1], R12[n+1], R12A[n+1], R12B[n+1], R13[n+1], R14[n+1], R2A[n+1], R3A[n+1],
R3A[n+1] , R3B[n+1];
double g, R2B[n+1], R2A[n+1], R3B[n+1], R3A[n+1], actcharge[n+1];
double pt, f3;
double stfn,sigma8,Prob,Prob2;
double chkfld;
double chkvalue;
int innerk;
double Pat[n+1], Ptc[n+1]; /*Prob. of tunneling(from:to)(a:activator,t:trap,c:conduction band)
in (n+1)th. section */
double Fn[n+1];  /* Flux in each section of the phosphor region*/
/*Flux in cathode Fnc and Flux in Anode Fna */
double nal[n+1], nah[n+1], nt2[n+1],dnt2;
double fltot,fl1,f12,fl3,f14,fl5,fl6,fl7,fl8,fl9,fl10,fl11;
double probb1, probb2, probb3, probb4, probb5, probb6, probb7, probb8, probb8, probb9,
probb10, probb11;
double dd1,dd2,dd3,dd4,dd5,dd6,dd7,dd8,dd9,dd10,dd11;
/*nal = density of electrons in lower energy level of the activator SrS:Cu */
/*nah = density of electrons in higher energy level of the activator SrS:Cu, nt2 = density of
electrons in the bulk trap level nal1 and nah1 are used in shallow_states function because you
dont want to use the updated values of nal and nah.*/
double c1,c3[n+1],c4[n+1],c5,c6; /* constants */
double nc1,nc2,nc3,nc4,nc5,nc6,nc7,nc8,nc9,nc10,nc11;
double na1, na2, na3, na4, na5, na6, na7, na8, na9, na10, na11;
double nca;  /* nc1 = shallowest interface state at cathode*/
double chrg;  /* nc11 = deepest interface state at cathode*/
            /* nsa = shallower interface state at anode*/
            /* nda = deeper interface state at anode */
double Lit[n+1]; /* Luminance in the ith. section at time t */
double Lt;  /* Luminance for the time slice */
double funcu;
long int j;
int i;
int z;
double lum_peak;  /* To find the peak luminence of the positive pulses */
double L1, L2;  /* To compare luminence peaks */
double Vapp;
double spacecharge[n+1], activatorcharge[n+1];
/* spacecharge = Nao-nal[i]-nah[i]-nt2[i] */
/* activatorcharge = Nao-nal[i]-nah[i] */
REFERENCES


Praveen Sivakumar, was born to Sivakumar Ramachandran and Vijaylakshmi Sivakumar, on January 9, 1979, in Chennai, India. He earned his Bachelor’s in Electronics and Communication Engineering from University of Madras in May 2000. He joined the Master’s program in Electrical and Computer Engineering at University of Kentucky in August 2000. He worked as a Research Assistant in the Electronic Devices Research Lab and Signal Processing Lab at University of Kentucky until August 2003.