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ROLE OF DIPOLES IN THE BULK PHOSPHOR LAYER IN THE ELECTROLUMINANCE MECHANISMS OF A.C. THIN FILM ELECTROLUMINESCENT DISPLAY DEVICES

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ABSTRACT OF DISSERTATION

Praveen Kumar Sivakumar

The Graduate School

University of Kentucky

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ABSTRACT OF DISSERTATION

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the College of Engineering at the University of Kentucky

By
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Lexington, Kentucky
Director: Dr. Vijay P. Singh
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University of Kentucky
Lexington, Kentucky
2008

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ROLE OF DIPOLES IN THE BULK PHOSPHOR LAYER IN THE ELECTROLUMINANCE MECHANISMS OF A. C. THIN FILM ELECTROLUMINESCENT DISPLAY DEVICES

The purpose of this dissertation is to advance the understanding of SrS-based a. c. thin film electroluminescent (ACTFEL) devices. The role of traps in the bulk phosphor layer in the light emission mechanism from ACTFEL devices is studied, characterized and modeled.

Experiments were performed to observe the response of the ACTFEL devices to tailored voltage excitations. A physical model was developed to describe the opto-electronic processes taking place in the phosphor; analytical equations were written and numerically simulated to plot the flux and luminance responses of the device to similarly tailored voltage excitations.

The voltage excitation parameters such as amplitude, rise times and fall times were varied both experimentally and in simulations and their effect on the opto-electronic response of the device was studied. Thermally stimulated luminance studies were performed to determine critical device parameters. Theoretical predictions matched the experimental data in a qualitative manner. A much improved quantitative accuracy is obtained when the role of dipoles in the EL mechanisms is incorporated into the model.

KEYWORDS: Electroluminescence; ACTFEL; SrS; Bulk Dipoles; Thermally Stimulated Luminance

PRAVEEN KUMAR SIVAKUMAR

February 28, 2008
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Dedicated to my
Advisor, Family and Friends
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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 radiative relaxation within a light-emitting center upon excitation by high-energy electrons. The electrons gain their energy due to acceleration in a high electric field. The light emitting centers are the dopants/activators introduced into the phosphor material.

1.2. History of Electroluminescence

Captain Henry Joseph Round first observed electroluminescence in 1907 when he discovered that yellow light was produced when a current was passed through a Silicon Carbide detector. O.V. Lossev from the Nijni-Novgorod Radio Laboratory in Russia confirmed this observation in 1923. Georges Distriau accidentally discovered electroluminescence in 1936 when he was working with ZnS compounds. In the 1950s, GTE Sylvania focused research efforts on powder EL phosphors for lighting applications. In 1967, Russ and Kennedy reported electroluminescence in a ZnS:Mn phosphor sandwiched between insulators. In 1969, Vlasenko and Popkov observed that thin film ZnS devices had much better characteristics than their powder counterparts. Soxman and Ketchpel demonstrated the possibility of matrix-addressing thin film electroluminescent (TFEL) displays with high luminance in the latter half of the 1960s, but unreliability of the devices remained a problem. In 1968, Aron Vecht demonstrated a direct current EL panel using powdered phosphors. In 1974, Inoguchi fabricated long-life devices and Mito demonstrated that these devices could be used for television imaging.
In 1981, Okamoto reported that rare-earth doped ZnS could be used in the phosphor layer of a TFEL device. The first commercial thin-film EL products were introduced by Sharp in 1983. Grid announced the first portable computer that used a 6-inch diagonal 320x240 pixel EL display panel. Subsequently, Sharp, Finlux and Planar International introduced half-page, 9-inch-diagonal yellow-emitting ZnS:Mn thin-film EL displays and 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].

In 1984, William Barrow from Planar International reported blue-green emissions from Strontium Sulfide doped with Cerium activators (SrS:Ce). In 1985, Shosaku Tanaka at Tottori University confirmed the findings of William Barrow and reported red emission from Calcium Sulfide (CaS). In 1988, Tanaka's group demonstrated white light emission from a TFEL display using a combination of SrS:Ce and SrS doped with Europium activators (SrS:Eu); they used the white light with color filters to demonstrate a full color display.

Sey-Shing Sun of Planar International demonstrated a SrS:Cu blue phosphor showing improved blue color and efficiency, with a wider color gamut in 1997. He demonstrated a true white color EL display using a SrS:Cu/ZnS:Mn multi-layer structure.

1.3. Display Technologies

1.3.1. Competing Technologies

Many different display technologies such as Cathode Ray Tube (CRT), Rear Projection TV and Flat Panel Displays (FPD) are commercially used today. CRTs have long life, good resolution, brightness and contrast controls, and color capabilities. However, they are bulky devices, require high voltage for operation and consume much more power than other competing technologies.
Three types of projection systems are used: CRT-based, Liquid Crystal Displays (LCD)-based and Digital Light Processing (DLP)-based. Projection TVs do not have the same image sharpness as other competing technologies and are expensive. However, the screen sizes can be up to 100 inches.

An alternative technology used widely in recent years is Flat Panel Display (FPD). LCDs are synonymous with FPD technologies. They are solid state devices and are rugged, lightweight, portable and consume less power for their operation. It is also possible to manufacture 12-70 inch full-color liquid crystal displays. They suffer from limited viewing angle, poor contrast ratios and loss of visibility under sunlight. LCDs find applications in computer and television displays.

Another flat panel display technology in use is Plasma Display. They have high luminance and contrast and modest resolution of 32 dots per inch but are expensive to manufacture. They are commonly used in large information screens and high-definition television applications.

Recently organic displays such as Organic Light Emitting Diode (OLED) devices are finding applications in cell phone, watch and small sized (less than 15”) displays because of their low-cost manufacturing advantages; efforts are underway to improve their luminous efficiency and lifetime.

### 1.3.2. ACTFEL Technology

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

1. Good contrast and can be used in very high ambient light.
2. High legibility because light is emitted from a sub-micron thick device and the pixel edges are sharp.
3. Lightweight devices and have wide viewing angle (>160°).
4. Very fast response time (few microseconds).
5. Do not require a backlight to function, unlike LCDs.

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 yet available 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. ACTFEL Phosphors and Dopants

The selection of phosphors and dopants for ACTFEL devices is very crucial as it influences the luminous output and efficiency of the device. The type of host phosphor selected can affect the lifetime of the devices and the brightness of the light emitted from the device; parameters such as band gap, transition states, lattice structure, light emission wavelength, valence matching, atomic size are taken into account when determining the dopant. Red emission is obtained by using CaS:Eu or ZnS:SM, P, yellow emission is obtained by using ZnS:Mn and blue emission is obtained by using SrS:Ce, SrS:Cu and SrS:Cu,Ag phosphors.

1.5. ACTFEL Display Research

SrS based ACTFEL devices with Cu activators [2]-[8] and with Ce activators [9]-[12] have been investigated for blue emitting displays. Efforts have been made to
understand the mechanism of light emission from these devices [7]-[27]. Electro-optical measurements have been performed on these devices [1, 28-29, 31-33] and luminance responses to various excitation pulses have been obtained.

These SrS based ACTFEL devices contain traps in the bulk phosphor, caused by the introduction of the dopant atoms such as Cu and Ce and the native defects in the SrS layer. These traps influence device operation and therefore, it is necessary to understand their properties. Two important characteristics are the depth of the trap level (from the conduction band of the phosphor), and the density of trap states. Various groups have studied the temperature dependence of the characteristics of these devices [8]-[9]. Simple models assuming a symmetrical device without space charge [17] and models that rely on the capacitive and leaky nature of the device with positive space charge in the phosphor layer [18] have been proposed. Models have been proposed to understand the high-field transport [24], excitation [21] and ionization [21, 27] mechanisms in these devices. Since late 1990s, based on the responses of the device to different excitation pulses, a more comprehensive model involving the traps has been proposed by Dr. Singh et. al. [2-3, 19, 23]. An important mechanism that has not been incorporated into any of these models yet is the effect of the dipoles in the bulk of the phosphor on the electro-optical mechanisms in the device. Incorporating the effect of the dipoles in these devices better models the processes occurring in the device, explains several unusual behaviors in the device and increases the accuracy of the model.

1.6. Motivation

The objective of this dissertation is to (1) understand, model and verify the electronic processes and luminance production mechanisms in a. c. thin film electroluminescent (ACTFEL) devices, (2) identify and evaluate the importance of various device parameters that affect the efficiency and luminance output of the devices, and (3) determine the optimal values of these parameters in order to maximize efficiency and luminance output. Better understanding of the processes in the host phosphor will result in more efficient blue emitting ACTFEL devices.
Towards this aim, experiments were performed to obtain the graphs of current flowing through the device and luminance output by the device. A physical model that describes the opto-electronic 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. The experimental and theoretical plots were compared and the results are presented and interpreted.
2. Theory

2.1. Physical Model for Opto-electronic Processes in ACTFEL Devices

When an external voltage is applied to the ACTFEL device (Figure 2.1), an electric field is set up across the phosphor. The structure of an ACTFEL device is shown in Figure 2.1. The electrons tunnel from the cathodic interface states (Process P1), accelerate in the high electric field in the phosphor bulk and are trapped at the anodic interface (Process P2). During their transit through the phosphor, they collide with the activators, causing excitation (Process P3) and ionization (Process P4), leading to dipole formation (Process P5) and subsequent relaxation (Process P6), resulting in light emission. Electrons released by ionization also travel through the phosphor and are trapped at the anodic interface. When the applied voltage is removed, the residual electric field aids in electron-tunneling from shallower anodic interface states at the anode. The ionized activators in the vicinity of the anodic interface recapture some of these electrons (Process P7); subsequent relaxation process causes light emission.
Figure 2.1: Schematic of SrS:Cu ACTFEL device showing the number of sections ‘n’, the total width of the phosphor ‘W_z’, the width of each section ‘W_x’ (=W_z/n) and the width of each insulator ‘W_i’

When a series of bipolar voltage pulses (Figure 2.2) is applied to this device in an experimental setup shown in Figure 3.1, current and luminance waveforms shown in curves 2 and 3 of Figure 4.1 are obtained during steady state operation. A sketch of voltage pulse shown in Figure 2.2 is used as an aid in the understanding of device operation.
At \( t = t_1 \) (Figure 2.2), the electric field in the phosphor is large enough to tunnel-eject electrons from the insulator-phosphor interface at the cathodic end and to accelerate them to a high enough energy to cause impact excitation of Cu activators; subsequent relaxation of activators produce light. The light emission during this time is called the leading edge (LE) luminance. As electrons travel from one end of the phosphor layer to the other, they impact the activators and cause excitation or ionization of these activators before reaching the anodic interface and getting trapped in the anodic interface states. The ionization process creates bulk space charge that causes spatial variations in the electric field. This spatial variation in the electric field plays an important role in understanding the behavior of SrS:Cu devices. After impact ionization, the released electron can end up in (i) the conduction band of SrS or, (ii) be trapped by a bulk trap in the vicinity of the activator, thus creating an electric dipole.

There is a minimum threshold field \( E_{\text{min}} \) needed to maintain the dipole; below this field, the dipole collapses. A field greater than \( E_{\text{min}} \) would be present at the leading edge when the dipoles are created, but when the bulk phosphor field drops below \( E_{\text{min}} \), the ionized activator recaptures the electron from its daughter trap and results in the annihilation of the dipole and the eventual emission of a photon when the activator
relaxes. The net phosphor field decreases substantially, just after the beginning of the trailing edge (BTE), when \( t = t_2 \). As a result, bulk dipoles collapse and photon emission leads to the luminance peak termed BTE.

As the applied voltage continues to decrease further, at some time \( t_3 \), the net electric field at the anodic end of the phosphor layer becomes zero. Thus, in the middle of the trailing edge (MTE), when \( t_3 < t < t_4 \), the net electric field is negative and electrons are therefore released from the shallow trap levels at the anodic interface states. These electrons recombine with the ionized activators near the interface and yield the luminance peak MTE.

It can be seen that the traps play a critical role in light-emission from SrS-based ACTFEL devices. Hence, the determination of trap energy levels using Thermally Stimulated Luminescence (TSL) technique is important to the design of efficient ACTFEL devices.
2.1.1. Mathematical Model for Opto-electronic Processes in ACTFEL Devices

Figure 2.3. shows the charge transfer taking place between various energy levels in the phosphor.

Figure 2.3. 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_{T}’ (Energy Level of the Bulk Trap) and ‘E_{C}’ (Energy Level of the Conduction Band of the Phosphor).

‘E_{AL}’ denotes the lower energy level of the activator; ‘E_{AH}’ denotes the higher energy level of the activator; ‘E_{T}’ 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 4.1eV. The energy difference between the lower and higher energy levels of the activator (Cu) is 2.75eV. The energy difference between the conduction band and bulk trap for different device configurations is obtained from Thermally Stimulated Luminescence (TSL) technique.
2.1.1.1. 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,

$$\Delta^2 \psi = -\rho/\varepsilon$$  \hspace{1cm} (1)

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

Region A \((0<x<W_1)\) is the insulator layer, region B \((W_1<x<W_1+W_Z)\) is the active SrS:Cu phosphor layer and region C \((W_1+W_Z<x<2W_1+W_Z)\) is the second insulator layer (Figure 2.1). To calculate the total electric field in the device, the electric field in each of these sections is first calculated.

**Region A:**

Assuming an ideal insulator, there is no space charge in the insulator. Hence, the electric field is constant in this region.

$$E_A(x) = C_1 \text{ Volts/cm}$$  \hspace{1cm} (2)

Hence, the voltage in region A is,

$$V_A(x) = C_1 x + C_2 \text{ Volts}$$  \hspace{1cm} (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,

$$\frac{dE}{dx} = \rho/\varepsilon$$  \hspace{1cm} (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,
\[ E_B(i,x) = C_3(i) + (q/\varepsilon_Z) \rho(i)(x-(W_1+(i-1)W)) \text{ Volts/cm} \]  
\( (5) \)

The voltage in \( i \text{-th} \) section is given by,
\[ V_B(i,x) = C_3(i) [x-(W_1+(i-1)W)] + C_4(i) + (q/2\varepsilon_Z) \rho(i)[x-(W_1+(i-1)W)] \text{ Volts} \]
\( (6) \)

where, ‘\( \rho(i) \)’ is the net positive charge density in section ‘\( i \)’, ‘\( \varepsilon_Z \)’ is the dielectric constant of SrS \((9.4*8.854*10^{-14} \text{ Farads/cm})\) and ‘\( q \)’ is the electronic charge \((-1.6*10^{-19} \text{ Coulombs})\).

**Region C:**

There is no space charge in the insulator, i.e. region C. Hence, the electric field is constant and is given by,
\[ E_C(x) = C_5 \text{ Volts/cm} \]
\( (7) \)

The voltage in region C is
\[ V_C(x) = C_5[x-(W_1+W_Z)] + C_6 \text{ Volts} \]
\( (8) \)

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

Assume that the transparent conductor Indium Tin Oxide (ITO) is at ground potential and a positive voltage is applied to the Aluminum back electrode.

At \( x = 0 \),
\[ V_A = 0 \]
\( (9) \)

At \( x = W_1 \),
\[ V_A = V_B \]
\( (10) \)
\[ D_B - D_A = q(n_{DC} + n_{SC} - n_{EQ}) \]
\( (11) \)

At \( x = W_1+W_Z \),
\[ V_B = V_C \]
\( (12) \)
\[ D_C - D_B = q(n_{DA} + n_{SA} - n_{EQ}) \]
\( (13) \)

At \( x = 2W_1+W_Z \),
\[ V_C = V_A \]
\( (14) \)
where, ‘D_A’, ‘D_B’, ‘D_C’ are the dielectric displacements in regions ‘A’, ‘B’ and ‘C’, and

\[ E_A = \frac{D_A}{\varepsilon_D}, \quad E_B = \frac{D_B}{\varepsilon_Z}, \quad E_C = \frac{D_C}{\varepsilon_D} \]  \hspace{1cm} (15)

where, \( \varepsilon_D = 7.9*8.85*10^{-14} \) 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:

\[ C_2 = 0 \]  \hspace{1cm} (16)

\[ C_3(1) = \frac{(\varepsilon_D C_1 - q(n_{SC} + n_{DC} - n_{EQ})/\varepsilon_Z)}{Volts/cm} \]  \hspace{1cm} (17)

\[ C_4(1) = C_1 W_1 Volts \]  \hspace{1cm} (18)

\[ C_3(i+1) = C_3(i) + \frac{(q/\varepsilon_Z)p(i)W}{Volts/cm} \]  \hspace{1cm} (19)

\[ C_4(i+1) = C_3(i)W + C_4(i) + \frac{(q/2\varepsilon_Z)p(i)W_x^2}{Volts} \]  \hspace{1cm} (20)

where, ‘i’ varies from 1 to ‘n’; ‘n’ is the total number of sections of the phosphor.

\[ C_5 = \frac{(C_3(n)\varepsilon_Z + q\rho(n)W - q(n_{DA} + n_{SA} - n_{EQ})/\varepsilon_D)}{Volts/cm} \]  \hspace{1cm} (21)

\[ C_6 = C_3(n)W + C_4(n) + \frac{(q/2\varepsilon_Z)p(n)W_x^2}{Volts} \]  \hspace{1cm} (22)

\[ V_A = C_5 W_1 + C_6 Volts \]  \hspace{1cm} (23)

### 2.1.1.2. Electron Tunneling from the Interface States

The electrons in the interface states tunnel by a mechanism known as “Fowler-Nordheim Tunneling”. It is a quantum mechanical process whereby the electrons tunnel through a thin barrier in the presence of a high electric field. A typical operating a. c. voltage of 120 V across a 1-micron thick phosphor sets up a high electric field of 1.2 MV/cm in the phosphor bulk. As a result, the electrons in the interface between the insulator and phosphor tunnel into the phosphor bulk. This process can be expressed mathematically as

\[ P_{DC} = a(mm)^{18} E_{DC}^{58} F^{-14} e^{-b(mm)^{12} E_{DC}^{12}} E_{DC}^{12} \]  \hspace{1cm} (24)

and
\[ P_{DC} = a \cdot (mm)^{18} \cdot E_{DC}^{38} \cdot F^{-14} \cdot e^{\frac{-b(mm)}{2} E_{DC}^{12}} \]  

(25)

where, \( P_{SC}(F) \) and \( P_{DC}(F) \) are the probabilities of field ionization from the interface states, \( F \) 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.

The total electron flux that tunnels out of the cathodic interface due to the applied electric field can be mathematically expressed as

\[ f = f_{OS} n_{SC} P_{SC} + f_{OD} n_{DC} P_{DC} \]  

(26)

where \( f_{OS} \) and \( f_{OD} \) are the occupancy constants of the shallower and deeper interface states; \( n_{SC} \) and \( n_{DC} \) are the density of electrons at the shallow and deep interface states.

**2.1.1.3. Charge Transfer and Luminance Processes in Phosphor Impact Excitation and Ionization Processes**

The tunnel-ejected electrons travel through the bulk of the phosphor and accelerate in the electric field present in the phosphor. These electrons gain energy and are termed “hot” electrons.

The phosphor is doped with a large density of activators (\( N_a \)). Since the activator has different physical and electrical properties than the host material, the introduction of activators in the host material results in defect traps. The trap density (\( N_t \)) is assumed to equal the activator density. The energy level of the traps is \( E_t \).

*The hot electrons, during their transit through the bulk, impact the activators, resulting in excitation or ionization.*

**2.1.1.3.1. Impact Excitation**

Upon impact by the hot electron, the electrons in the lower energy level of the activator (\( E_{AL} \)) gain energy and are transferred to a higher level within the activator (\( E_{AH} \)). This process can be mathematically expressed as
where $R_I$ is the rate of electron transfer from the lower energy level of the activator to the higher level, $f$ is the flux of incoming electrons, $f_i(E)$ is the fraction of incoming hot electrons that have enough energy to impact excite electrons from the level $E_{AL}$ to $E_{AH}$, $l(x,t)$ is the density of electrons in the lower energy level of the activator (and hence its spatial and temporal dependence), $R$ is the radius for impact (defined as the radius around an activator that a hot electron must pass through to cause an impact process) and $A$ is the area of the device.

2.1.1.3.2. Impact Ionization

If the incoming hot electron has sufficient energy, then it can knock an electron out of the activators, thereby ionizing it. The hot electron can knock out electrons from either the lower energy level of the activator, or the higher energy level of the activator or both. The electron that has been knocked out of the activator can end up in 2 places:

1. it can be trapped in the neighboring defects, or

2. it can flow through the phosphor along with the hot electrons, gaining energy due to the accelerating electric field and cause further impact ionization or excitation processes.

2.1.1.3.3. Impact Ionization from the Lower Activator Level to the Neighboring Traps

Upon impact by the hot electron, the activator is ionized and the electrons in the lower energy level of the activator ($E_{AL}$) are knocked out from the activator and end up in the neighboring traps. These traps are in close vicinity of the activator (since the traps are caused due to the defects formed in the host lattice when the activators are introduced); this results in a positively charged activator and a negatively charged trap in close proximity, i.e. a dipole. This process can be mathematically expressed as

$$R_{2A} = ff_2(E) f_3(E) l(x,t) \pi R^2 A, \quad \text{if} \quad l(x,t) < \rho_T$$  \hspace{1cm} (28)
$$R_{2A} = ff_{2}(E) f_{3}(E) \rho_{T} \pi R^{2} A, \quad \text{if} \quad l(x,t) > \rho_{T}$$  \hspace{1cm} (29)$$

where $R_{2A}$ is the rate of the impact ionization from lower level activator states to bulk traps, $f$ is the flux of incoming electrons; $f_{2}(E)$ is the fraction of electron flux that has enough energy for impact ionization of electrons; $\rho_{T}$ is the trap density; $f_{3}(E)$ is the fraction of electrons which are impact ionized to the trap level $E_{T}$; $R$ is the radius for impact (defined as the radius around an activator that a hot electron must pass through to cause an impact process); $l(x,t)$ is the density of electrons in the lower energy level of the activator and $A$ is the area of the device.

2.1.1.3.4. Impact Ionization from the Higher Activator Level to the Neighboring Traps

Upon impact by the hot electron, the activator is ionized and the electrons in the higher energy level of the activator ($E_{AH}$) are knocked out from the activator and end up in the neighboring traps. This results in a positively charged activator and a negatively charged trap in close proximity, i.e. a dipole. This process can be mathematically expressed as

$$R_{3A} = ff_{2}^{1}(E) f_{3}^{1}(E) u(x,t) \rho R^{2} A, \quad \text{if} \quad u(x,t) < \rho_{T}$$ \hspace{1cm} (30)$$

$$R_{3A} = ff_{2}^{1}(E) f_{3}^{1}(E) \rho_{T} \rho R^{2} A, \quad \text{if} \quad u(x,t) > \rho_{T}$$ \hspace{1cm} (31)$$

where $R_{3A}$ is the rate of the impact ionization from higher level activator states to bulk traps, $f$ is the flux of incoming electrons; $f_{2}^{1}(E)$ is the fraction of electron flux that has enough energy for impact ionization of electrons; $\rho_{T}$ is the trap density; $f_{3}^{1}(E)$ is the fraction of electrons which are impact ionized to the conduction band; $R$ is the radius for impact (defined as the radius around an activator that a hot electron must pass through to cause an impact process); $u(x,t)$ is the density of electrons in the higher energy level of the activator (and hence its spatial and temporal dependence) and $A$ is the area of the device.
2.1.1.3.5. Impact Ionization from the Lower Activator Level to the Conduction Band

Upon impact by the hot electron, the activator is ionized and the electrons in the lower energy level of the activator \((E_{AL})\) are knocked out from the activator and end up in the conduction band. These electrons then travel through the phosphor, accelerating in the electric field in the bulk, gaining energy and impacting activators (causing further excitation and ionization processes) before getting trapped at the other interface. This process can be mathematically expressed as

\[
R_{4A} = \mathcal{f} f_2(E) \left( 1 - f_3(E) \right) l(x,t) p R^2 A, \quad \text{if} \quad l(x,t) < \rho_T \tag{32}
\]

\[
R_{4A} = \mathcal{f} f_2(E) \left( 1 - f_3(E) \right) \rho_T p R^2 A, \quad \text{if} \quad l(x,t) > \rho_T \tag{33}
\]

where \(R_{4A}\) is the rate of the impact ionization from lower level activator states to bulk traps, \(f\) is the flux of incoming electrons; \(f_2(E)\) is the fraction of electron flux that has enough energy for impact ionization of electrons; \(\rho_T\) is the trap density; \((1-f_3(E))\) is the fraction of electrons which are impact ionized to the conduction band \(E_C\); \(R\) is the radius for impact (defined as the radius around an activator that a hot electron must pass through to cause an impact process); \(l(x,t)\) is the density of electrons in the lower energy level of the activator and \(A\) is the area of the device.

2.1.1.3.6. Impact Ionization from the Higher Activator Level to Conduction Band

Upon impact by the hot electron, the activator is ionized and the electrons in the higher energy level of the activator \((E_{AH})\) are knocked out from the activator and end up in the conduction band. These electrons then travel through the phosphor, accelerating in the electric field in the bulk, gaining energy and impacting activators (causing further excitation and ionization processes) before getting trapped at the other interface. This process can be mathematically expressed as

\[
R_{5A} = \mathcal{f} f_2(E) \left( 1 - f_3(E) \right) u(x,t) p R^2 A, \quad \text{if} \quad u(x,t) < \rho_T \tag{34}
\]

\[
R_{5A} = \mathcal{f} f_2(E) \left( 1 - f_3(E) \right) \rho_T p R^2 A, \quad \text{if} \quad u(x,t) > \rho_T \tag{35}
\]
where \( R_{5A} \) is the rate of the impact ionization from higher level activator states to bulk traps, \( f \) is the flux of incoming electrons; \( f^d(E) \) is the fraction of electron flux that has enough energy for impact ionization of electrons; \( p_T \) is the trap density; \( (1-f^d(E)) \) is the fraction of electrons which are impact ionized to the conduction band; \( R \) is the radius for impact (defined as the radius around an activator that a hot electron must pass through to cause an impact process); \( u(x,t) \) is the density of electrons in the higher energy level of the activator (and hence its spatial and temporal dependence) and \( A \) is the area of the device.

### 2.1.1.3.7. Field assisted tunneling from lower energy level of the activator to the bulk traps

Due to the high electric field present in the device (a few MV/cm), the electrons can tunnel from the activator to the traps. The process of tunneling from the lower energy level of the activator \( (E_{AL}) \) to the traps can be mathematically written as

\[
R_{2B} = \begin{cases} 
  l(x,t) P_{EAL1} & \text{if } l(x,t) \leq p_T \\
  p_T P_{EAL1} & \text{if } l(x,t) > p_T 
\end{cases}
\]  

where, \( P_{EAL1} \) is the probability of field assisted tunneling from \( E_{AL} \) to \( E_1 \).

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

where, \( R_{2B} \) is the rate at which electrons undergo field assisted tunneling from lower level activator states to bulk traps, \( F_i \) 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; \( p_T \) is the density of empty bulk traps and is given by:

\[
p_T = n_{t0} - n_{t2}
\]

where, \( n_{t0} \) is the density of bulk traps in the phosphor layer; \( n_{t2} \) is the electron density at trap level \( E_1 \).
2.1.1.3.8. Field assisted tunneling from higher energy level of the activator to the bulk traps

The process of tunneling from the higher energy level of the activator \((E_{AH})\) to the traps can be mathematically written as

\[
R_{3B} = u(x,t) P_{EAHE1} \quad \text{if } u(x,t) \leq p_T \tag{36a}
\]

\[
R_{3B} = p_T P_{EAHE1} \quad \text{if } u(x,t) > p_T \tag{36b}
\]

where, \(P_{EALEH}\) is the probability of field assisted tunneling from \(E_{AH}\) to \(E_1\).

\[
P_{EHE1} = a \left( \frac{m^{1/8}}{m^{1/8}} \right) E_{AH}^{5/8} F_i^{1/4} \exp \left( - \left( b \frac{m}{m^*} \right)^{-1/2} \frac{E_{AH}^{3/2}}{F_i} \right) \tag{37}
\]

where, \(R_{3B}\) is the rate at which electrons undergo field assisted tunneling from lower level activator states to bulk traps, \(F_i\) is the electric field in the \(i^{th}\) section; \(E_{EAHE1}\) is the energy gap between \(E_{AH}\) and \(E_1\); \(m\) and \(m^*\) are the mass and effective mass of electron respectively; \(a\) and \(b\) are constants associated with the barrier; \(p_T\) is the density of empty bulk trap.

Luminance is the ratio of the luminous intensity in a given direction of infinitesimal elements of a surface containing the point under on a plane perpendicular to the given direction. The luminance is measured by a photometer. The luminance is a photometric term indicating the radiated power in terms of human eye sensitivity. The physical measure of the luminous intensity is \(\text{cd/m}^2\). It is also expressed as \(\text{fL (foot-lamberts)}\).

\[
1 \text{fL} = \frac{1}{\pi} \text{ cd/} \text{(ft)}^2 = 3.426 \text{ cd/m}^2 \tag{38}
\]

2.2. Thermally Stimulated Luminescence

The device under test (DUT) is cooled to very low temperature and the temperature is increased linearly. The increasing temperature increases the vibrations of the crystal lattice; the effect of this phenomenon is to eject the electrons out of the trap states in the device; subsequent relaxation produces luminance. By measuring this
stimulated luminescent as a function of temperature, the energy levels of the traps in the
device can be estimated.

Equation (39) follows from the kinetic analysis and is used to extract energy
levels from the TSL response.

\[ I = n_0 s e^{(-E_t/kT)} \left( \frac{(l - 1) s}{\beta} \int_{T_0}^{T} e^{(-E_t/kT)} dT' + 1 \right)^{-(l(l-1)/2)} \quad (39) \]

The integral is evaluated as,

\[ \int_{0}^{T} e^{(-E_t/kT)} dT' = T e^{(-E_t/kT)} \sum_{j=1}^{l} \left( \frac{kT}{E_t} \right)^j (-1)^{j-1} j! \quad (40) \]

where \( E_t \) is the trap energy, \( T \) is the temperature, \( \beta \) is the rate of heating, \( n_0 \) is the number
of trapped carriers, \( l \) is the order of the trapping process and \( s \) is the escape frequency.

If the bulk of the phosphor is thought to contain ‘N’ multi-energy level traps, the
TSL curves due to N multiple independent traps is obtained by using Equation 41.

\[ I(T) = \sum_{j=1}^{N} I_j(T) \quad (41) \]

The data obtained experimentally and theoretically are fit, by minimizing the
mean square error between the two curves.

\[ \sqrt{\frac{\sum_{i=1}^{N} (y_i - x_i)^2}{N}} \quad (42) \]
3. Experimental and Numerical Procedures

3.1. Experiments

3.1.1. Display Testing System

The display testing system was developed to test ACTFEL devices for display panel applications and record acquired data for further analysis. The present system allows testing devices in a.c. mode and recording four different waveform parameters: Applied Voltage, Current through the device, Light Output Response and Charge flowing through the Device. The system is configured to capture one data point every microsecond. The maximum possible voltage is in the range +500/-500V, but for available ACTFEL devices, +160/-160V is typically used.

3.1.2. System Hardware

The schematic representation of the display system is shown in Figure 3.1. A computer running Display Testing System Software Version 1.0 under LABVIEW 6 and developed in our labs controls the system. The computer has a GPIB interface card connected through the GPIB bus to the oscilloscope, signal waveform generator and Monochromator. The oscilloscope can record four channels: Applied Voltage to the Device, Voltage on the Sense Capacitor, Output of the Photo Multiplier Tube and Current Output.

The maximum output signal of the waveform generator is 10V. In order to bring the output to the voltage required for device operation, a custom amplifier was built based on the Apex PA89 operational amplifier. Two power supplies connected in series as Master Slave configuration are used to supply power to the amplifier. The range of sensitivity of the photomultiplier tube was 185-900nm.
Figure 3.1: Schematic of Displays Testing System Hardware
The layout of a typical ACTFEL device is shown below:

![Figure 3.2: Typical Device Layout](image)

A layer of ITO was coated on a glass substrate. The insulator layer, made up of Aluminum Titanium Oxide (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 Barium Tantalate (BTO)/ATO 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 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.
3.1.3. System Software

The Display Testing System software was executed in Labview 6.0 graphical environment. It could be run in Single Measurement Mode, Excitation Voltage Sweep Mode and Wavelength Sweep Mode. More information can be found in [12].

3.1.4. Experimental Procedure

1. Spring loaded probes were used to make contact to the ACTFEL device
2. The voltage excitation pulses were tailored by changing various parameters including Rise Time, Fall Time, On Time, Amplitude, Half Period, No. of Pulse Cycles, Transient Wait Time, Notch Start Time, Notch Length and Notch Depth.
3. The starting voltage, final voltage, number of steps and the voltage step were selected; these pulses were amplified and applied to the device.
4. The current flowing through the device was amplified using a coil of 100 loops and measured as a function of time.
5. The light emitted by the device was passed through a spectrometer and specific wavelengths were passed through a photomultiplier tube; the resultant signal was measured as a function of time.
6. The results were plotted using Microsoft Excel/MATLAB.

3.2. Simulations

3.2.1. Simulation Procedure

A mathematical model for the opto-electronic processes in SrS:Cu ACTFEL devices was developed, and a C program was written to verify the validity of the model. The C program incorporated the various mathematical equations that described the method of luminance production in SrS:Cu ACTFEL device.

The results were compared with the experimentally obtained data. For the purpose of simulation, the phosphor layer was divided into 100 sections. The simulation time increment $\Delta t$ was chosen to be 50 ns. This choice of $\Delta t$ was made after varying $\Delta t$ over a
wide range and studying the effects on the results of the simulation. Field and charge in each section were then assumed to be constant over this small time interval \( \Delta t \) and all the processes of interest were calculated based on this assumption. Transition rates were computed during each interval and the space charge, field and current were updated every 50 ns. The simulation procedure is illustrated in the flowchart in Figure 3.3.
Start

Open data files to store results of simulations

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

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

1

Calculate electric field in all ‘n’ phosphor sections using the equations.

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

Is field at anode < 0?

Yes

Calculate flux tunneling from anodic interface states and update population at anodic interface

No

Flux travels from the cathodic interface towards anodic interface

Is flux from anodic interface > flux from cathodic

Yes

Flux travels from the anodic interface towards cathodic interface

No

Calculate light output from single section

Calculate rates of charge transfer between various energy levels according to equations.

Update population at energy levels according to equations.
Calculate flux and 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

Yes

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

Yes

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

No

No

Stop

Figure 3.3. Simulation Flowchart
As shown in the flowchart above, the data files (in which the simulated voltage, current and luminance curves were stored) were opened. Initial state conditions were set before the simulation was actually run. The voltage was “built” according to the required amplitude and rise and fall times and the resultant electric field was calculated in every section. This electric field caused the electrons to tunnel out of the interface states. The resultant population at the interface was updated to reflect this change. The electrons thus ejected from the interfaces caused opto-electronic processes described in the model. When these electrons reach the other end, they were trapped at the other interface and relax from the shallow interface state to the deep interface state subsequently.

Due to the opto-electronic processes taking place in the bulk of the phosphor, the electron densities at the lower and higher energy levels as well as the trap and conduction band density vary and they are calculated as per the equations described in Section 2. Thus, the flux generated at every section adds to the flux ejected from the interface or the previous section. As a result of the activator relaxation, luminance is produced in the device and is calculated using the equation described in Section 2.

The simulation procedure adopted is described below [12]:

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 100. 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 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 2). 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. The resulting flux initiated the opto-electronic processes in the subsequent sections.

7. The luminance in each section was computed and the total luminance was computed by summing up light emitted from each section.

8. 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.

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

10. 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 $k^{th}$ section was exchanged with that in the $(n-k)^{th}$ section where ‘$k$’ varied from 1 to ‘$k/2$’.

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

12. 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/MATLAB.
3.2.2. 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 opto-electronic processes were described, is given below [12].

1. **prog.c**

The processes described in Section 2 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 [12]:

   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 2). 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 probability 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. 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 Ba₂TaO₆) was calculated in this routine. The electrons tunneled out of the anodic interface due to the applied electric field by Fowler-Nordheim tunneling. The probability 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. bulk_phosphor()

The bulk_phosphor() routine was used to describe the opto-electronic processes taking place in the phosphor. The luminance contribution of each section was calculated. The rate equations (described in Section 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 opto-electronic processes in the current section was added to the flux generated in the section under consideration and the resulting flux caused the opto-electronic 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 2).

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 2).

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\textsuperscript{th} section in the phosphor was swapped with the (n-k)\textsuperscript{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 ($V_{\text{max}}$), 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 ($E_l$, $E_{11}$, $E_{\text{AL}}$, $E_{\text{AH}}$, $E_T$),
f. device parameters such as the density of activators in phosphor ($N_{ao}$), the densities of interface states ($n_{cl}$, $n_{cl1}$, $n_{al}$, $n_{al1}$), the dielectric constants ($e_o$, $e_d$) 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

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

The values of device parameters and constants used for simulations in this dissertation are as follows:

\[ E_{sc} = \text{shallower interface state energy level} = 0.4 \text{ eV}; \ E_{dc} = \text{deeper interface state energy level} = 0.74 \text{ eV}; \ E_t = \text{bulk trap level} = 0.4 \text{ eV}; \ E_H = \text{higher activator energy level} = 0.9 \text{ eV}; \ E_L = \text{lower activator energy level} = 3.6 \text{ eV}; \text{ all energy levels are referenced from the bottom of the conduction band of SrS}; \ n_{sc} = \text{electron density in the shallower interface energy level} = 5 \times 10^{14} \text{ cm}^{-2}; \ n_{dc} = \text{electron density in the deeper interface energy level} = 10^{16} \text{ cm}^{-2}; \ N_{t0} = \text{bulk trap concentration} = 10^{19} \text{ cm}^{-3}; \ N_{a0} = \text{activator concentration} = 10^{19} \text{ cm}^{-3}; \ E_{min} = \text{Electric field below which dipoles collapse} = 1.3 \text{ MV·cm}^{-1}; \ \tau_d = \text{activator relaxation time} = 10 \times 10^{-6} \text{ s}; \ \nu_{th} = \text{thermal velocity} = 2.33 \times 10^7 \text{ m/s}. \]
cm·sec$^{-1}$; $v_{sat} =$ saturation velocity $= 10^7$ cm·sec$^{-1}$; $S_{nt} =$ capture cross section area of the activator $= 10^{-16}$ cm$^2$.

These values were arrived at by experimentation, references to standard values and refinement during simulations.

3.3. Thermally Stimulated Luminescence

3.3.1. Experimental Procedures

The experimental setup to obtain Voltage-Current-Luminescence (V-I-L) characteristics of the ACTFEL device as a function of time is shown in Figure 3.1. The DUT was subjected to voltage pulse excitations using the waveform generator-amplifier setup and the resulting current was fed to the digital oscilloscope. The light output by the device was collected by means of an optical cable fiber, was fed to the photomultiplier tube, then to the oscilloscope and finally to the computer.

A preset train of voltage pulses was applied to the device and the resulting current and luminance waveforms were collected. These were plotted as a function of time and were collectively labeled V-t, I-t and L-t waveforms. The V-I-L waveforms were plotted during the initial transient, and after the DUT had reached steady state. To obtain the L-V curves, a Minolta luminance meter was used to measure the intensity of the light emitted by the device as a function of pulse amplitude.

For the TSL measurements, the DUT was cooled to 10 K with a CTI cryopump [8]. The sample was excited with approximately 10 mW of 260-nm ultraviolet radiation from a 1000 W xenon lamp. The excitation wavelength was selected with a spectral energy monochromator and a 4 cm$^2$ spot size. The samples were excited from the SrS:Cu or Al$_2$O$_3$/SrS:Cu side of the film. The radiation was turned off and luminescence allowed to decay for up to 1 h. The sample temperature was then increased at a linear rate of 15 °C/min. The TSL emission was collected with a Pritchard model 1980B equipped with a GaAs photomultiplier tube that has a spectral response from 300 to 800 nm. For the temperature range above 450 K, filters were used to reduce the blackbody signal from the
holder. All TSL spectra were taken at least twice to ensure the accuracy of the features as well as determine if the incident radiation damaged the sample [8].

3.3.2. Numerical Procedures

A program was written in C to simulate the kinetic processes described by equations in Section 2.2. Traps at a single energy level $E_1$ were initially assumed and the code was executed. Eqn. 41 was used to fit the experimental TSL data of SrS ACTFEL devices and the values for energy level, $E$ and $s$ were obtained.
4. Results and Discussion

The field, current and luminance in these devices have been investigated and the results are discussed in the following sub-sections. The role of the dipoles in the bulk of the phosphor is incorporated into the model and the simulations are performed taking into account the effect of these dipoles.

4.1. Identifying, Modeling and Evaluating the Role of Dipoles in the Bulk Phosphor Layer in the EL Mechanisms

1. The charge carrier transport involves the following processes: (1) tunneling from the semiconductor-insulator interface states, (2) impact ionization from the activators, and (3) tunneling from the activators and traps to the conduction band of the semiconductor. The importance of these processes in determining the output characteristics of the device has been evaluated.

2. There are dipoles in the bulk region of the SrS based ACTFEL devices; the origin of the dipoles is the activator-trap pair (formed by impact ionization of the activators). The effect of dipoles on the efficiency has been studied and modeled; the results of the experiments are compared with the simulated results that were based on the model incorporating the role of bulk traps in the opto-electronic processes. Bulk traps play an important role in determining the efficiency and luminance output of the SrS based ACTFEL devices. The effect of the bulk traps (charge capture-release processes, influence on the local electric field, effect on tunneling, ionization and luminance processes) has been investigated and modeled; optimal concentration of the bulk traps has been numerically evaluated to realize more efficient devices.

3. Activator ionization plays an important role in the device operation. The impact of activator ionization on the efficiency of the device has been evaluated. The effect of trapping and subsequent recapture processes on the luminous efficiency of the device has been evaluated numerically.

4. Activator concentration plays an important role in determining the efficiency of the ACTFEL device. The effect of varying activator concentration has been studied.
5. It has been observed experimentally that the luminance waveforms possess 3 distinct peaks; these have been named beginning edge, beginning of trailing edge and middle of trailing edge peaks. The cause of the 3 peaks had been hypothesized by Singh et al [3]. These hypotheses have been verified both qualitatively and quantitatively by numerically simulating the mathematical model. The beginning of trailing edge peaks is attributed to the dipole collapse processes in the bulk of the phosphor and is included in the model.

6. Experiments show that the trailing edge peak occurs even with a small reduction in applied voltage; this was not explained by earlier hypothesis or existing literature. The dipole collapse causes one of the trailing edge peaks and the recapture of electrons from the anodic interface by the charged activators and subsequent relaxation produces the other trailing edge peak. The experimental V-I-L characteristics are compared with the simulated V-I-L characteristics to verify this hypothesis.

4.2. Experimental and Numerical Results

A typical V-I-L (Voltage-Current-Luminance) plot is explained in Section 4.2.1; next, V-I-L plots at different voltages, different rise and fall times, different activator and trap concentrations, different interface state populations and different threshold field for dipole collapse are explained and the role of bulk dipoles is evaluated.

4.2.1. V-I-L Characteristics

An alternating trapezoidal voltage pulse with amplitude 123 V, rise time = 100 μs, fall time = 100 μs and pulse width = 250 μs, with time between pulses = 4550 μs was applied to SrS:Cu,Ag ACTFEL device; the resulting current and luminance response was plotted. The analytical model was simulated using the identical drive parameters.

The steady state response to a train of bipolar trapezoidal voltage pulses of pulse width 250 μs, rise time and fall time of 100 μs, frequency of 100 Hz and amplitude of 123 V shows relatively weak BTE and MTE (Figure 4.1). The calculated current and luminance in steady state (199th pulse) are shown in Figure 4.2.
Figure 4.1: Experimental V-I-L characteristics for SrS:Cu ACTFEL device for $V_{app}=123V$
Figure 4.2: Simulated voltage, current and luminance waveforms for a SrS:Cu,Ag ACTFEL device showing Leading Edge (LE), Beginning of the Trailing Edge (BTE) and Middle of the Trailing Edge (MTE) peaks for $V_{\text{amp}} = 123$ V.

The responses in Figure 4.2 are similar in nature to the experimental current and luminance waveforms of Figure 4.1. Both figures exhibit three luminance peaks, first at the leading edge (LE), second at the beginning of the trailing edge (BTE) and third at the middle of the trailing edge (MTE). Figure 4.3 shows the detail of Figure 4.2 during the leading edge, including the electric fields at the cathodic and anodic interfaces.

In Figure 4.1, we note that the current reached its maximum value earlier than the applied voltage. This can be understood in terms of the electric fields plotted in Figure 4.3.
From Figure 4.3, we see that the electric field at the cathodic interface and the current reach their maximum at approximately the same time, $t_1 \approx 100 \, \mu s$. Also, at this time, the electric field at the anodic interface (and in the bulk phosphor layer) is smaller and is continuing to decrease. As a result, the electron flux generated by impact excitation and ionization of activators is decreasing; hence, the total phosphor current starts to decrease after $t_1$.

In Figs. 4.1 and 4.2, the BTE is attributed to the collapse of dipoles [2] [3]. These dipoles are formed by activators that have lost an electron (through impact ionization) to “their” daughter traps. A minimum field ($E_{\text{min}}$) in the device is necessary for the dipoles to exist. In the case shown in Figure 4.2, most of the dipoles that formed during the leading edge “survived” just until after the trailing edge started (and the net field reduced below $E_{\text{min}}$). **However, in general, dipoles can start to relax before, or after the trailing edge in voltage has started.** Mini-peaks in the simulated luminance waveform are caused by the collapse of dipoles in different sections of the phosphor layer, at different times.
The third luminance peak (MTE) occurs in the middle of the trailing edge, when backflow or reverse tunnel current appears [3].

In order to understand the nature of electric field variation in the phosphor layer (Figure 4.3), note that at the end of the previous (198th) pulse, there was (i) residual charge at each interface, (ii) residual positive charge in the bulk due to ionized activators and (iii) non-uniform, residual field created by the above charges. Just after the 199th voltage pulse starts to rise, a constant displacement current, resulting from the capacitive nature of the device and proportional to dV_{amp}(t)/dt, appears while the electric field across the phosphor increases uniformly. At time t_3 (≈ 70 μs) in Figure 4.3, the electric field threshold (E_{th}) is reached and electrons at the cathodic interface tunnel-eject into the conduction band, creating an electron flux that will eventually travel across the entire length of the phosphor layer. When the electric field threshold is reached, the field along the phosphor is relatively high, so that most electrons, after tunneling, acquire high kinetic energy, and these traveling electrons tend to impact-ionize more activators (and do not get trapped by residual ionized activators from the last pulse). This is a current-multiplication process that causes the positively-charged new anodic interface to be neutralized well before the negative charge at the new cathodic interface is significantly decreased; thus, the anodic field starts to decrease (t_4) before the cathodic field does (t_1).

After the voltage reaches its maximum at t = t_1, the electric field at the cathode drops to a value below the threshold (E_{th}), tunnel-ejection stops and impact-ionization practically disappears. However, field-ionization continues because this process is more likely to occur when the activator is in its excited state than when it is in its ground state. Thus, during the few tens of microseconds after t_2, when a significant number of activators are still in their excited state, conduction current persists, along with light output, which is also proportional to the excited activator population. The delay between the luminance peak and the current peak is attributed to the delay caused by the trapping of electrons by the ionized activators.

The measured and the simulated peak currents are 72.5 mA/cm² (experimental) and 66.42 mA/cm² (theoretical) for V_A = 123 V. Experimental and theoretical charge transferred per pulse were 2.75 μC/cm² and 2.26 μC/cm². Peak experimental and simulated luminance values for V_A = 123 V case was 531 cd/m² and 49150 cd/m².
respectively. Total experimental and simulated luminance values for $V_A = 123$ V case was $6.2 \text{ cd/m}^2$ and $561.2 \text{ cd/cm}^2$ respectively. It is clear that the luminance actually harvested is much less than the luminance available in the device. This is attributed to the following factors:

1. Only 10% of the light generated in the device is emitted through the glass side; the rest is emitted along the edges of the device, after undergoing multiple reflections in the device [16, 34].

2. Concentration quenching and activator aggregation [30, 32].

3. Model does not account for the distance an electron must travel (after each impact) to regain enough energy for impact excitation/ionization [24].

4. Quenching because of neighbor defects.

4.2.2. Luminance-Voltage (L-V) Characteristics

The device was excited with trapezoidal waveforms with varying amplitudes but fixed rise and fall times (=100 $\mu s$); the luminance response was collected and plotted. The simulations were performed with the same excitation voltage parameters and the luminance response was collected and plotted.

Figs. 4.4 and 4.5 show the experimental and simulated luminance-voltage characteristics. This L-V curve features a threshold voltage $V_{th}$ below which little luminance is emitted, a steeply rising characteristic above threshold, and finally a saturation region. The threshold voltage $V_{th}$ is defined as the voltage applied to the device that produces a luminance of 1 cd/m$^2$. Above a threshold voltage, luminance is produced. This threshold voltage is the voltage required to set up the electric field in the device that causes conduction current to flow. The experimental $V_{th}$ is 90 V and the simulated $V_{th}$ is 115 V. Losses occurred during luminance collection during measurements because of total internal reflections.
Figure 4.4: Experimental Total Luminance-Voltage (cd/sq.m) characteristics of the SrS:Cu ACTFEL device with rise time = fall time = 100 μs.

Figure 4.5: Simulated Total Luminance-Voltage (cd/sq.m) characteristics of the SrS:Cu ACTFEL device with rise time = fall time = 100 μs.
Figure 4.6: Experimental log(Total Luminance)-Voltage (cd/sq.m) characteristics of the SrS:Cu ACTFEL with rise time = fall time = 100 μs.

Figure 4.7: Simulated Total log(Luminance) -Voltage (cd/sq.m) characteristics of the SrS:Cu ACTFEL device with rise time = fall time = 100 μs.
Figure 4.8: Experimental Peak Luminance-Voltage (W/sq.m) characteristics of the SrS:Cu ACTFEL device with rise time = fall time = 100 μs.

Figure 4.9: Simulated Peak Luminance-Voltage (W/sq.m) characteristics of the SrS:Cu ACTFEL device with rise time = fall time = 100 μs

Above the threshold voltage, Luminance rises rapidly because of increased transfer charge in the phosphor layer. The sharp increase in luminance is due to the
tunnel injection of electrons from trap states at the phosphor layer/insulating layer interface.

*It is observed that the ratio of total luminance emitted per pulse at various voltages between experimental and simulated values is almost constant.* The experimental luminance is lesser than simulated luminance because certain factors have not been incorporated into the model as explained in section 4.2.1. The number of activators in the device plays a crucial role in determining the amount of light emitted from the device; this is discussed in detail in Section 4.2.6.3.

*The luminance produced by the device increases as voltage increases and saturates at a critical voltage;* beyond this voltage, any increase in voltage does not result in a substantial increase in luminance. This is because, the excitable activators have all been exhausted at this critical voltage and any further increase in voltage increases the flux of “hot” electrons but not the number of light producing transitions (Figure 4.4). The number of excitable activators present at any time is tracked more accurately by taking into account the continuous formation and annihilation of dipoles in the bulk of the phosphor, its effect on the localized electric field and ionization mechanisms.

### 4.2.3. Efficiency-Voltage (η-V) Characteristics

The efficiency of the EL device is defined as the luminance produced by the device per watt of input power applied to the device. The device was excited with trapezoidal waveforms with varying amplitudes but fixed rise and fall times (=100 μs); the luminance and current responses were collected and plotted. The simulations were performed with the same excitation voltage parameters and the luminance and current responses were collected and plotted.

Figs. 4.10 and 4.11 show the experimental and simulated efficiency-voltage characteristics.
Figure 4.10: Experimental Efficiency-Voltage (lm/W) characteristics of the SrS:Cu ACTFEL with rise time = fall time = 100 μs.
As the applied voltage increases, both the current and luminance increases. However, the luminance stops increasing after a critical voltage (Figure 4.10) because the device has been exhausted of excitable activators; hence, *even though the applied voltage tunnel-ejects the electrons from the interface, thereby increasing the input power to the device, the luminance output from the device does not increase proportionally.*

After the electrons have tunneled out of the interface states, any further increase in voltage would not increase the conduction current substantially (though it will increase the rate of impact ionization from the activators or traps) but will influence BTE luminance because of the greater electric field in the device. The experimental efficiency (Figure 4.10) is lower than the simulated efficiency (Figure 4.11) since the experimental luminance is much lower than the simulated luminance (Figure 4.4, 4.5).
4.2.4. Charge-Voltage (Q-V) Characteristics

The device was excited with trapezoidal waveforms with varying amplitudes but fixed rise and fall times (=100 μs); the current response was collected and plotted. The simulations were performed with the same excitation voltage parameters and the luminance response was collected and plotted.

Figure 4.12, 4.13 show the experimental and simulated charge transferred per pulse for different voltages and constant rise and fall times (100 μs) for the SrS:Cu device.
Figure 4.12: Experimental Total Charge-Voltage ($\mu$C/sq.cm) characteristics of the SrS:Cu ACTFEL with rise time = fall time = 100 $\mu$s.
Figure 4.13: Total Charge - Voltage (µC/sq. cm) characteristics of the SrS:Cu ACTFEL device with rise time = fall time = 100 µs.

Figure 4.14: Experimental Peak Current (mA/sq. cm) characteristics of the SrS:Cu ACTFEL device with rise time = fall time = 100 µs.
It is observed that the transferred charge increases as voltage increases until a certain voltage and then, the charge transferred is nearly constant. The total charge transferred through the device to the other interface can decrease as a result of 3 factors:

1. The cathodic interface has been exhausted of all the electrons due to the increased ejection rate at large electric field setup in the device due to the higher voltages applied to this device.

2. An increasing voltage sets up a higher electric field in the phosphor layer; as the electric field increases, the flux of electrons tunnel-ejected from the interface increases. The charge is transferred between the interfaces due to this applied field. This transferred charge sets up an electric field in the device that opposes the applied field. The positively charged ionized activators increase this internal electric field; the net field decreases as a result. This results in fewer electrons tunneling from the interfaces.

3. The rate of electrons that leave the activator due to ionization is decreased due to the dynamic nature of the electric field in the device and hence, the total transferred
charge decreases [2]. The incorporation of the dipole formation and collapse processes in the model describes the local ionized activator population and electric fields more accurately.

Thus, the voltage amplitudes were varied over a wide range of values and the theoretical values of peak luminance, peak current, total luminance and total charge transferred were compared with the experimental values; the results were nearly proportional for different device excitation parameters.

4.2.5. Thermally Stimulated Luminescence to Determine Trap Densities and Levels

4.2.5.1. Depths of Trap Levels

The normalized experimental and simulated TSL intensity as a function of temperature for the SrS:Ce ACTFEL device is shown in Figure 4.16. A dominant peak at 111 degrees Kelvin is observed in the experimental TSL characteristic. Using Eqns. (1)-(3), this peak was identified as an intrinsic trap state in the phosphor bulk of SrS:Ce at a depth of 0.18 eV below the conduction band of SrS. The escape frequency, which is a measure of the frequency with which the electrons strike the sides of the potential well of the trap and the reflection coefficient, was calculated to be $1 \times 10^7$ s$^{-1}$. For this calculation, only the dominant peak in the experimental data was considered. Even though several smaller peaks are present in Figure 4.16, these are thought to be insignificant as far as device operation is concerned. Earlier, in a similar fashion, an intrinsic trap level in the SrS:Cu device was measured to be at 0.4 eV below the conduction band and its escape frequency was calculated to be $3.23 \times 10^5$ s$^{-1}$ [8].
4.2.5.2. Effect on Device Performance

A value of 0.4 eV for the trap depth level, $E_T$ was substituted in the theoretical equations describing the device operation [12] and the $I$-t and $l$-t values were calculated. The simulated VIL waveforms in steady state are shown in Figure 4.2. Figure 4.2 shows the theoretical current, and luminance outputs obtained from the simulation program [4], [14] with the following set of values:

- $n_{SC} = 5 \times 10^{13} \text{ cm}^{-3}$; $n_{DC} = 10^{15} \text{ cm}^{-3}$; $f_0 = f_{od} = 1$; $n_{a0} = 10^{19} \text{ cm}^{-3}$; $n_{a0} = 10^{19} \text{ cm}^{-3}$; $E_{min} = 0.8 \text{ MV cm}^{-1}$; $\tau_d = 0.05 \times 10^{-6} \text{ s}$; $a = 9 \times 10^{10}$; $b = 1.49 \times 10^{8}$; $v_{th} = 23.3 \times 10^6 \text{ cm sec}^{-1}$; $v_{sat} = 1.0 \times 10^7 \text{ cm sec}^{-1}$; $r = 1 \times 10^{-8} \text{ m}$; $S_{nt} = 10^{-16} \text{ cm}^2$; $\gamma = 1/\tau_2 = 1/1 \times 10^{-5} \text{ s}^{-1}$; $\Delta E_{E1EC} = E_C - E_1 = 0.4 \text{ eV}$; $f_2(E) = 2 \cdot f_2(E)$; $f_3 = 0.6$; $f_3 = 0.6$; $\Delta E_{E1E1E1} = E_1 - E_{AL} = 3 \text{ eV}$; $E_{SC} = 0.4 \text{ eV}$; $E_{DC} = 0.673045 \text{ eV}$.

Figure 4.16: Normalized experimental and calculated TSL Intensity vs. Temperature characteristics for a SrS:Ce ACTFEL device
The corresponding experimental current and luminance waveforms are shown in Figure 4.1. Experimental and theoretical waveforms are qualitatively similar in as much that they both exhibit three distinct luminance peaks. These peaks, termed LE, BTE and MTE occur, respectively, at (1) the leading edge (LE) of the applied voltage pulse, (2) the beginning of the trailing edge, (BTE) of the applied voltage pulse, and (3) the middle of the trailing edge (MTE) of the applied voltage pulse.

At the leading edge of voltage in both Figs. 4.1 and 4.5, current reaches its peak value just a little before the luminance does. This indicates that impact ionization of activators and trap states play an important part in device operation [4]. The light emission mechanism is at least partially due to the ionization of Cu activators and subsequent trapping of low energy electrons. If impact excitation had been the only light emission mechanism, then current and light would have peaked at the same time as they do in ZnS:Mn ACTFEL devices [15].

4.2.6. Effect of Varying Drive and Device Parameters

The values of certain important device and drive parameters were varied over a wide range and numerical simulations were performed. These parameters include driving voltage amplitude, rise and fall times of the driving voltage pulse, activator concentration in the phosphor, depth of interface states at both the cathodic and anodic interfaces, threshold electric field for dipole collapse in the bulk phosphor and the probability of dipole formation. The values of each of these parameters were varied one at a time so that the effect of each of these parameters on the VIL characteristics could be observed and interpreted. For all simulations in Sections 4.2.6.1 to 4.2.6.5, the starting point was the constants listed above in Section 4.2.5.2.

4.2.6.1. Effect of Varying Voltage Amplitudes ($V_{amp}$)
In this study, $V_{\text{amp}}$ was varied from 90 V to 165 V. Experimental and simulated voltage, current, and luminance waveforms for $V_{\text{amp}}$ values of 123 V, 127 V and 132 V are shown in Figs. 4.17, 4.18, 4.19 and Figs. 4.20, 4.21, 4.22 respectively.

![Graph showing experimental voltage, current, and luminance waveforms](image)

**Figure 4.17:** Experimental voltage, current and luminance waveforms for a SrS:Cu,Ag ACTFEL device showing a Leading Edge (LE), Beginning of the Trailing Edge (BTE) and Middle of the Trailing Edge (MTE) peaks for $V_{\text{amp}} = 123$ V.
Figure 4.18: Experimental Voltage, current and luminance waveforms for a SrS:Cu,Ag ACTFEL device for $V_{amp}=127$ V
Figure 4.19: Experimental Voltage, current and luminance waveforms for a SrS:Cu ACTFEL device for $V_{amp}=132$ V
Figure 4.20: Simulated voltage, current and luminance waveforms for a SrS:Cu,Ag ACTFEL device showing a Leading Edge (LE), Beginning of the Trailing Edge (BTE) and Middle of the Trailing Edge (MTE) peaks for $V_{amp} = 123 \, \text{V}$. 
Figure 4.21: Simulated Voltage, current and luminance waveforms for a SrS:Cu ACTFEL device for $V_{amp}=127$ V
Figure 4.22: Simulated Voltage, current and luminance waveforms for a SrS:Cu ACTFEL device for $V_{amp}=132$ V

Similar behavior in SrS:Cu,Ag ACTFEL devices has also been reported by Huttl et. al [15]. At low voltages ($V_{amp} < 123$V), no appreciable conduction current is seen. The net electric field in the phosphor is far too low to make the ejected electrons numerous or energetic enough to impact excite the activators due to low applied voltage; yet it is high enough to field-ionize the activators, and thus, create dipoles. BTE luminance is emitted when the activator-trap dipoles relax.

At $V_A=123$ V, conduction current and LE and MTE appear. As the voltage amplitude is increased both current and luminance increase.

In Figs 4.18, 4.19, 4.21 and 4.22, we note that the current reached its maximum value much earlier than voltage.

The electric field in the device increases as the voltage applied to the device increases. When the threshold electric field for tunneling from interface states is reached, electrons tunnel out of the cathodic (1) insulator-phosphor interface and reach the anodic
interface. On their path, the electrons collide with the activators and ionize them. As a result, there is a positively charged interface (1) (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 (2) (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 (1), the rate at which impact ionization occurs in the phosphor and the rate at which an electron is transferred from one interface to another.

The electric field at the cathodic interface and the current reach their maximum at the same time \( t_1 \). Cathodic field then clamps and remains constant until \( t = t_2 \) when the applied voltage stops rising. After \( t_2 \), cathodic field decreases. Between \( t_1 \) and \( t_2 \) the rate of increase of cathodic field due to the rising voltage is exactly counteracted by the rate of increase in the internal field at the cathode. However the electric field at the anodic interface (and in the bulk phosphor layer) is smaller and in continuing to decrease. As a result the electron flux from impact ionization of activators is also decreasing and hence the total phosphor current starts to decrease after \( t_1 \) even though the cathodic field does not decrease until \( t_2 \). Thus, under the assumption of an infinitely large interface state electron population, experimental observations of current peaking before the voltage can serve as evidence for ionization of activators or traps in the bulk phosphor layer. If the interface state electron population is not infinitely large, and is subject to exhaustion, then, of course, the reduction in current between \( t_6 \) and \( t_7 \), in spite of constant cathodic field, could be attributed to reduced tunnel current resulting from reduced interface electron population.

In Figs. 4.17 and 4.18, the leading edge luminance peak trail the current peak by a few microseconds. This expected delay is attributed to the time needed for the relaxation of impact excited electrons to the lower level as well as the recombination of impact-ionized electrons. On the other hand, in the luminance characteristics in Figs. 4.18, 4.19, 4.21, 4.22 we find that the luminance reached its maximum value earlier than current. This is explained in terms of exhaustion of excitable activators:
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. However, the number of activators available for impact decreases with each impact process. Hence, at some later time, a smaller number of unexcited and un-ionized activators are available for impact. Hence, any subsequent increase in flux has a reduced effect on the luminance emitted by the device. Consequently, luminance reaches its maximum value before current and begins to decrease even though current continues to increase.

*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.* The third luminance peak (MTE) occurs in the middle of the trailing edge. At this time, reverse tunnel current also appears. This reverse tunnel current arises when the net field at the anodic interface is high enough to cause tunneling of electrons at the anode back into the conduction band. As these electrons go into the conduction band they can cause luminance through two processes: i) impact excitation of activators followed by relaxation. This process does not have a low probability of occurrence since the “reverse” field is high enough to cause tunneling, it should also be high enough to cause impact excitation ii) recapture of electrons by ionized activators. Although in either case, a reverse tunnel current should be observed, it is small compared to the “forward” tunnel and displacement currents.

The transferred charge density increases linearly as a function of voltage above the threshold voltage, which is seen more explicitly shown in linear L-V and Q-V curves for SrS:Cu device driven at 123V for the experimental and 123V in simulations. *The luminance is proportional to the transferred charge density within the phosphor layer, so that an increase in the transferred charge is bound to improve the luminance.* The excitation probability (the function of the energy received by the hot electrons from the electric field) of the luminescent centers by the hot electrons should be improved.

The luminance produced by the device increases as voltage increases and saturates at a critical voltage; beyond this voltage, any increase in voltage does not result in a substantial increase in luminance. The excitable activators have all been exhausted at
this critical voltage and any further increase in voltage increases the flux of “hot” electrons but not the number of luminance producing transitions. For this reason, as the applied field stops increasing and the built-in counter-field keeps increasing due to field-assisted-ionization of activators, the field in the phosphor near the anode (which is lower in magnitude) falls below the $E_{\text{min}}$ necessary to maintain dipoles. Consequently, *dipoles collapse and emit luminance in the form of a “shoulder” in the LE peak*. The “shoulder” is clear for $V_{\text{amp}} = 132$ V. If most of the possible dipoles get formed even for the reference $V_{\text{amp}} = 160$ V case, a higher $V_{\text{amp}}$ would not significantly increase the number of formed dipoles. After the voltage ramp-up, about the same number of dipoles exist in the phosphor layer for the reference case and for higher $V_{\text{amp}}$ conditions. *Having the same number of dipoles in these cases, but with dipole collapse starting earlier in the pulse for the higher $V_{\text{amp}}$ cases, dipole collapse will also end earlier, resulting in shorter duration of $BTE$ at $V_{\text{amp}} = 132$ V.*

MTE is not significantly affected when $V_{\text{amp}}$ goes above the reference case, although it is absent for $V_{\text{amp}} = 117$V. However, for the sufficiently high $V_{\text{amp}} = 132$ V, “reverse” tunnel current appears, which results from electrons at the anodic interface back-flowing into the conduction band after the applied field is removed and the net field at the anode becomes “negative”. For higher applied fields, a higher built-in reverse field is built to keep the cathodic field below $E_{\text{th}}$.

**4.2.6.2. Effect of Varying Rise and Fall Times of the Applied Voltage Pulses ($V_R$ and $V_T$)**

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 30 $\mu$s to 150 $\mu$s and the current and luminance response of the device was collected and plotted. Simulations were performed by applying voltages of constant amplitude (=160V), and varying rise and fall times from 30 $\mu$s to 150 $\mu$s; the flux and luminance response was collected and plotted [12]. The experimental and simulated results are presented below.
4.2.6.2.1: Driving voltage = 160V; Rise Time = Fall Time = 30μs.

Experimentally obtained VIL characteristics are shown in Figure 4.23 and the simulated VIL characteristics are shown in Figure 4.24.

*Figure 4.23: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 30μs*
Simulated VIL Characteristics for Driving Voltage of 160V at Rise time = 30 microseconds

Figure 4.24: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 30μs
4.2.6.2.2: Driving voltage = 160V; Rise Time = Fall Time = 60μs.

Experimentally obtained VIL characteristics are shown in Figure 4.25 and the simulated VIL characteristics are shown in Figure 4.26.

*Figure 4.25: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 60μs*
Figure 4.26: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 60μs
4.2.6.2.3: Driving voltage = 160V; Rise Time = Fall Time = 100μs.

Experimentally obtained VIL characteristics are shown in Figure 4.27 and the simulated VIL characteristics are shown in Figure 4.28.

Figure 4.27: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 100μs
Figure 4.28: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 100\(\mu\)s
4.2.6.2.4: Driving voltage = 160V; Rise Time = Fall Time = 110μs.

Experimentally obtained VIL characteristics are shown in Figure 4.29 and the simulated VIL characteristics are shown in Figure 4.30.

![Graph showing experimentally obtained VIL characteristics](image)

*Figure 4.29: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 110μs*
Figure 4.30: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 110μs
4.2.6.2.5: Driving voltage = 160V; Rise Time = Fall Time = 130μs.

Experimentally obtained VIL characteristics are shown in Figure 4.31 and the simulated VIL characteristics are shown in Figure 4.32.

![Figure 4.31: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 130μs.](image-url)
Figure 4.32: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 130µs
4.2.6.2.6: Driving voltage = 160V; Rise Time = Fall Time = 150μs.

Experimentally obtained VIL characteristics are shown in Figure 4.33 and the simulated VIL characteristics are shown in Figure 4.34.

Figure 4.33: Experimentally obtained VIL characteristics for driving voltage of 160V with rise time and fall time of 150μs.
Figure 4.34: Simulated VIL characteristics for driving voltage of 160V with rise time and fall time of 150μs.

The conduction current flowed much earlier for shorter rise times and had fallen to zero by the time the voltage had reached its maximum value. Since charges are transferred to the other interface rapidly, internal electric field builds up very quickly in the phosphor. This increase in internal electric field decreases the net electric field in the phosphor, 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.

The luminance curves exhibited interesting characteristics. The LE luminance peaked at almost the same time instant as the current peaked and it had a pronounced shoulder. The BTE peak was absent for shorter fall times. The MTE luminance peak was larger and sharper for shorter fall times. 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). 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. Thus, the shape of the MTE luminance is also influenced by the fall time of the driving voltage.

4.2.6.3. Effect of Varying Activator Concentration ($N_{a0}$)

The activator concentration ($N_{a0}$) plays an important role in the phenomenon of light emission from the ACTFEL devices. To simulate the effect of the activator concentration on the luminance characteristics, and hence efficiency characteristics, $N_{a0}$ was varied between $10^{18}$ cm$^{-3}$ and $3 \times 10^{19}$ cm$^{-3}$ (the number of traps in the bulk of the phosphor equaled the number of activators) and the simulations were performed.

Figs. 4.35, 4.36, 4.37, 4.38 and 4.39 show the simulated voltage, current and luminance (VIL) waveforms for the $N_{a0}$ values of $9.5 \times 10^{18}$, $9.67 \times 10^{18}$, $9.97 \times 10^{18}$, $1 \times 10^{19}$ and $1.1 \times 10^{19}$ cm$^{-3}$ respectively.

![Figure 4.35: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for $V_{amp} = 123$ V for $N_{a0} = 9.5 \times 10^{18}$ cm$^{-3}$](image-url)
Figure 4.36: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for $V_{amp} = 123$ V for $N_a = 9.67 \times 10^{18}$ cm$^{-3}$.

Figure 4.37: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for $V_{amp} = 123$ V for $N_a = 9.997 \times 10^{18}$ cm$^{-3}$.
Figure 4.38: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for $V_{amp} = 123$ V for $N_{a0} = 1.0 \times 10^{19}$ cm$^{-3}$
For a lower Na₀ value of 9.67x10¹⁸ cm⁻³, the luminance waveform exhibits the first trailing edge pulse (BTE), but no leading edge (LE) pulse or the MTE pulse. This is because the activator concentration is far too low to intercept the electron flux. Yet, a few activators are field-ionized and BTE luminance is emitted when the dipoles relax.

At the higher activator concentration value of 9.997x10¹⁸ cm⁻³ and 10¹⁹ cm⁻³ (Figure 4.36), the luminance waveform exhibits all three pulses. At the leading edge, luminance peaks after current, as is normal in sufficiently doped ACTFEL display devices (Figure 4.5).

At the yet higher activator concentration level of 1.1x10¹⁹ cm⁻³, the number of dipoles is large enough that BTE peak in luminance is enlarged and merges with the MTE peak. Mini-peaks associated with dipole collapse appear even before the voltage amplitude is reduced at trailing edge.
In order to increase the luminance from the device, it appears that increasing \( N_{a0} \) is the best solution; it should be noted that there is an upper limit. This is because of the following reasons:

1. The activators get ionized, creating bulk charge and reducing the field near the anode; this, in turn, reduces the luminance from the device at higher values of \( N_{a0} \).
2. Upon impact-excitation, the kinetic energy of the electron is transferred to the activator, so that the activator ends up in the excited state. Hence, the impacting electrons need to gain enough kinetic energy before they effectively impact-excite an activator. If the activator concentration is too high, electrons keep colliding with activators before they have gained enough kinetic energy. When this happens, most of the kinetic energy of the electron is dissipated as heat, so that the electron loses its energy without causing impact-excitation. This phenomenon is known as activator quenching.

4.2.6.4. Effect of Varying Interface State Depth \( (E_{d,0}) \)

In the model, based on experimental results, we have assumed that only two levels of interface states exists and that electrons relax from the shallow \( (E_1) \) into the deep states \( (E_{11}) \). The analytical model was numerically simulated using the standard values of the parameters, only varying the depth of the deep cathodic and anodic interface states interface state, \( E_{11} \), from 0.72 eV to 0.76 eV. The depth of the shallow interface state, \( E_1 \), was kept constant at 0.4 eV. *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 relaxation time constant from shallow to deep states was 50 ns and the time between successive voltage pulses was 5000\( \mu \)s. The relaxation time from deep to shallow is short enough that when a pulse is applied, all the electrons reside in the deep interface states. For this reason, \( E_{11} \) plays an important role in determining the current and luminance characteristics during the first part of the applied pulse.
Figure 4.40: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for \( V_{\text{amp}} = 123 \, V \) for \( E_{11} = 0.72 \, eV \)

Figure 4.41: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for \( V_{\text{amp}} = 123 \, V \) for \( E_{11} = 0.75523 \, eV \)
The nature of resulting variations in current and luminance [16] was similar in nature to variations seen with voltage amplitude. Current and luminance waveforms were found to be critically dependent on the depth of the interface states energy level; deviations as small as 1% from its nominal value resulted in large variations in current, field and luminance. More details on the effects of varying this parameter can be found in [12].

As $E_{11}$ increases, the time delay between the current peak and the voltage peak ($t_{IV}$) diminishes. As $E_{11}$ increases, the threshold voltage increases. Conduction current appears later and peaks later in time. Thus, $t_{IV}$ decreases as $E_{11}$ is increased; at $E_{11} = 0.755233$ eV, $t_{IV} = 0$. $t_{IV}$ remains at zero for higher values of $E_{11}$. The depth of interface states variation can make the current peak shift with respect to the voltage peak.

For high values of $E_{11}$ (0.72 eV), the applied voltage is not strong enough to cause electrons to tunnel from the interface states. As $E_{11}$ decreases and the electrons tunnel out more easily, conduction current and luminance appear. Also, dipoles are formed even
when there is not an appreciable amount of impact excitation ($E_{11} = 0.72$ eV). When $E_{11}$ is within “reach” of the applied field, when conduction current and LE appear, there is also a certain amount of backflow, so that MTE is present whenever LE is. When $E_{11}$ is even shallower ($E_{11} = .76$ eV), dipole collapse takes place so early in the pulse that LE appears to have a secondary peak, a “shoulder”. This is because more charge is transferred; more ionization occurs due to a larger number of electrons flowing across the phosphor and more bulk charge is created. Bulk charge causes a differential between the electric field at the cathodic and anodic sides of the phosphor layer, so that the phosphor section near the anode goes under $E_{\text{min}}$ sooner, causing dipoles to collapse earlier.

### 4.2.6.5. Effect of Varying Threshold Electric Field for Dipole Collapse ($E_{\text{th}}$)

In the model, upon electron impact-excitation, activators can lose an electron to the conduction band or to a nearby trap. When the latter happens, if the electric field is high enough (above $E_{\text{min}}$), the positively charged activator and the negatively charged trap are separated by the electric field by virtue of their opposite charges (if in the right position, otherwise would be brought together). A dipole will be created, which will collapse when the electric field falls below the minimum required for keeping the activator and trap sufficiently apart ($E_{\text{min}}$). When the electric field goes below $E_{\text{min}}$, the trap gets close to the activator and the electron is transferred to excited energy level of the activator, where it relaxes and emits light.

Thus, the activator-trap dipoles collapse when the electric field goes below the threshold field $E_{\text{min}}$ [1]. This leads to radiative relaxation in the activator and consequently, the BTE luminance.

Numerical simulations were performed by varying the threshold electric field for dipole collapse in the bulk phosphor between 0.3MV/cm and 1.7MV/cm. Its effect on the luminance and current characteristics of the ACTFEL device was studied.

Figs. 4.43, 4.2.2 and 4.45 show the voltage, current and luminance waveforms for the $E_{\text{min}}$ values of 0.4 MV/cm, 0.6 MV/cm and 1.7 MV/cm respectively.
Figure 4.43: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for $V_{amp} = 123$ V for $E_{min} = 0.4$ MV/cm

Figure 4.44: Simulated voltage, current and luminance waveforms for a SrS:Cu ACTFEL for $V_{amp} = 123$ V for $E_{min} = 1.7$ MV/cm
It is observed for higher $E_{\text{min}}$ values, the BTE luminance peak is absent. This is because all dipoles have already collapsed before the voltage begins to decrease at the trailing edge. *It has been observed that many SrS:Cu,Ag ACTFEL devices does not exhibit a BTE luminance peak.*

According to the model [2, 12, 15], dipoles form at the leading edge when the voltage and net field are rising. They collapse after the voltage pulse has reached its maximum and the net field is decreasing; this is because a minimum threshold field ($E_{\text{min}}$) is necessary to sustain the dipoles in the bulk of the phosphor. The formation process begins later for higher values of $E_{\text{min}}$ and the collapsing process begins earlier.

It is observed that the luminance waveform exhibits a jagged waveform between the LE and MTE luminance peaks. 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 peak has a jagged waveform.

The electric field at the anode had fallen below 0.3 MV/cm before the applied voltage started to decrease and hence, the dipoles near the anode begin to collapse at this point. Subsequently, the dipoles in the sections between the cathode and the anode begin to collapse and finally, the dipoles at the cathode collapse.

*The value of $E_{\text{min}}$ depends on the physical distance between the activator and its “daughter” trap and the angle between their line-of-sight and the electric field lines.*

*It was observed that varying the threshold electric field at which dipoles collapse had a significant impact on the BTE luminance.* 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. 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. The total area under the BTE luminance peaks was constant.

The BTE luminance is attributed to collapse of dipoles in the phosphor and subsequent relaxation of the electrons within the activators. 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. The electric field varies both in time and space within the
phosphor. 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.

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 luminance. Hence, the BTE peaks have a jagged waveform.

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

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.

As can be seen in figures 4.45 and 4.46, decreasing the number of sections of phosphor during the simulations results in greater accuracy (at the expense of the computation time) and the resulting L-T waveform is less jagged; this is because the local electric field changes more gradually in the device and hence, the number of dipoles collapsing at any time is smaller (due to smaller section widths).
Figure 4.45: Simulated luminance vs. time waveforms for a SrS:Cu ACTFEL for n=100 sections

Figure 4.46: Simulated luminance vs. time waveforms for a SrS:Cu ACTFEL for n=1000 sections
5. Conclusion

1. Simulations of field, current and luminance in SrS based ACTFEL devices incorporating the role of dipoles in the bulk of the phosphor revealed the physical mechanisms by which several “unusual” behaviors in device characteristics are produced. The model accounted for the beginning of trailing edge luminance, its occurrence in certain devices and under certain drive conditions, light emitted by the device and the efficiency of the device. These features were observed experimentally and cannot be explained by the earlier, more simplistic models of the past.

2. The model predicted that under certain different operating conditions current in the phosphor can be decreasing during a time interval when the electric field at the cathodic interface is clamped at a constant value.

3. A match between the measured and the simulated peak currents (72.5 mA/cm$^2$ (experimental) and 66.42 mA/cm$^2$ (theoretical)) was obtained for $V_A = 123$ V for SrS:Cu,Ag devices.

4. The experimental and theoretical charge transferred per pulse were 2.75 $\mu$C/cm$^2$ and 2.26 $\mu$C/cm$^2$.

5. The peak experimental and simulated luminance values for $V_A = 123$ V case were 531 cd/m$^2$ and 49150 cd/m$^2$ respectively. Total experimental and simulated luminance values were 6.2 cd/m$^2$ and 561.2 cd/cm$^2$ respectively. The variation in the luminance is accounted for by concentration, activator and defect quenching, light emission from the edges due to multiple internal reflections, activator aggregation and some assumptions regarding mean free path in the model.

6. The voltage amplitudes were varied over a wide range of values and the theoretical values of peak luminance, peak current, total luminance and total charge transferred were compared with the experimental values. The theoretical calculation and experimental measurement results track each other in a proportional manner, for different device excitation parameters.
7. The effects of voltage amplitude, activator concentration, interface energy levels, and critical field for dipole collapse were studied. These simulations showed that secondary (after the main peak) luminance peaks can be produced by: i) electron “backflow” from the cathodic interface when the magnitude of the applied voltage pulse decreases and by ii) ionized activators recapturing “their” electron from a neighboring trap.

In summary, the model is able to predict all expected as well as “unusual” features in the response of the SrS based ACTFEL device. Furthermore, the generalized model developed in this dissertation can be applied to other ACTFEL devices (such as yellow-emitting ZnS:Mn devices) which have simpler device operation mechanisms than SrS:Cu, Ag/SrS:Ce device investigated here.
Appendix A: List of Constants (constants.h)

/* model parameters */

#define TAU2 10E-06 /* relaxation time */

#define radiu 4.999E-8 /* Radius for impact */

#define fnew3 0.60 /* fraction impact ionized from lower energy level of the activator to the traps */

#define fprimenew3 0.60 /* fraction impact ionized from higher energy level of the activator to the traps */

#define delta_Tdipole 5E-06 /* time for dipole collapse */

#define a1 9.0E+10

#define b1 1.49E+08

#define a2 9.0E+10

#define b2 1.49E+08

#define K 1 /* correction factor = k0.k1.k2.k3.k4 */

#define B 4.2E-19 /* light emitted in Joules for 1 transition from higher to the lower energy level of the activator */

#define sigma5 0.4E-3 /* fitting parameter for R5 */

#define sigma9 1E-3

/*********************************************/

#define delta1 1.0E-15

#define beta1 1.0E-17
# define beta2 1.0E-6

# define beta1p 2.53E-13

# define beta2p 2.53E-2

# define G1 1.0E-14

# define tau1 1.75E-6

# define delta_Tl 1000E12

# define E11 3

# define delta_T 0.05E-06 /* simulation time interval */

# define Ts 9000 /* simulation duration */

/**********************************************************/
/* applied voltage parameters */

# define Vs 120.0 /* applied voltage */

# define RISE_TIME 2000 /* rise time for the applied voltage pulse */

# define FALL_TIME 7000 /* fall time for the applied voltage pulse */

# define NO_OF_PULSES 200 /* total number of pulses */

/**********************************************************/
/* phosphor parameters */

# define Nt2 1.00E19 /* density of traps */

# define Nao 1.00E19 /* density of activators */
# define Nc  3.14E+18 /* density of states in the conduction band */

# define ez  83.19E-14 /* dielectric constant of phosphor */

# define ed  69.92E-14 /* dielectric constant of insulator */

# define n  100 /* number of sections of phosphor */

# define Wz  0.513E-4 /* total width of the bulk phosphor layer */

# define Wx  0.513E-6 /* width of each of the 'n' sections of phosphor */

# define W1  1.525E-5 /* width of each insulator */

/********************************************************************************
/* depth of interface states */
#define E1  0.4 /* depth of the shallowest interface state */
#define E2  0
#define E3  0
#define E4  0
#define E5  0
#define E6  0
#define E7  0
#define E8  0
#define E9  0
#define E10 0
#define E11 0.743155 /* depth of the deepest interface state */

/* density of interface states */
#define N1  5E+14 /* density of the shallowest interface state */
#define N2  0
#define N3  0
#define N4  0
#define N5  0
#define N6  0
# define N7  0
# define N8  0
# define N9  0
# define N10 0
# define N11 10.0E+15 /* density of the deepest interface state */

/* physical constants */

# define m 9.1E-31
# define m_star 2.28E-31
# define mobility 100
# define SIGMA2  1.0E-8
# define SIGMA1  5.0E-11
# define SIGMA3 4.0E-5
# define Sn  1.0E-17
# define Snt  1.0E-16
# define Vth  2.33E+07
# define Vsat 1.0E+07
# define Eb 1.06
# define Etc 0.4
# define KT 0.0259
# define ALPHA 2.0E-16
# define Neq  5.0E+15

# define Nto  0

# define q  -1.6E-19

# define Snd  2.2E-17
Appendix B: List of Variables (variables.h)

FILE *Macrofile;
FILE *FluxFile;
FILE *Infofile;
FILE *VILfile;
FILE *EIfile;
FILE *Scaledfile;
FILE *Timefile;
FILE *nahvsT;

double e_cathode[100000], e_anode[100000];
double max_e_cathode, max_e_anode, tot_luminance, totalflux;
double fnew1;
double nahct;
double tot_lit;
int flux_point;
double flux_disp;
double tot_flux_unscaled;
double tot_flux_scaled;

    *Nahpt;
    /*These are all file-pointers*/

    *Rhox2000vsT, *Ex3000vsT, *Rhox3000vsT,
    *Ex4000vsT, *Rhox4000vsT, *Ex4500vsT, *Rhox4500vsT; /* Electric Field as a
    function of space */

typedef struct phosphor_slice {
    double c3;
}
double Fn;  /* Flux in each section of the phosphor region*/
   /* Flux in cathode Fnc and Flux in Anode Fna */
double nal, nah, nt2;
double actcharge;
double Lit;  /* Luminance in the ith. section at time t */
double condnband;
double spacecharge;  /* spacecharge = Nao-nal[i]-nah[i]-nt2[i] */
} phosphor_t;
phosphor_t phos[n+2];  /* most arrays only use up to n+1; Fn, JFn need up to n+2 */

double g;
double pt, f3;
double stfn;
double chkfld;

double chkvalue;
double innerk;
double max_flux_disp;
double setr;
int dum_count;
double tot_charge;
/*Prob. of tunneling(from:to)(a:activator,t:trap,c:conduction band)*/
/* in (n+1)th. section */
double total_charge;
double dnt2;
double fltot,fl1,fl2,fl3,fl4,fl5,fl6,fl7,fl8,fl9,fl10,fl11;
double probb1,probb2,probb3,probb4,probb5,probb6,probb7,probb8,probb9,probb10,probb11;

double dd1,dd2,dd3,dd4,dd5,dd6,dd7,dd8,dd9,dd10,dd11;
double c1,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;
double chrg;   /* nc11 = deepest interface state at cathode*/
double Lt ; /* Luminance for the time slice */
double funcu;
/* int ctr_i; WRD: unused */
long int j;
long int t;
double Lum[100000];
double Vol[100000];
double Flu[100000];
long int run_t;
double max_lum,max_v,max_flux;
int t_i;
int z;
int flux_direction;
double fld_tunnel;
double lum_peak;
/* To find the peak luminence of the positive pulses */

double L1, L2;    /* To compare luminence peaks */

double Vapp;

double fnew2,fprimenew2,fnew1;

int set_tunnel;
Appendix C: ACTFEL Simulation Code (main.c)

/***************************************************************************
********************
Title:  actfel.c  
Using 2 interface states
Author: Praveen Sivakumar

***************************************************************************/

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

void init(void);
void exchange(void);
void driver(void);
void anodic_interface(void);
void write_scaled_file(void);
void constants(void);
void cathodic_tunneling(void);
void bulk_phosphor(void);
void shallow_states(void);
void cathodic_interface(void);
void anodic_interface(void);
void anodic_tunneling(void);

int main (int argc, const char * argv[]) {
    Infofile = fopen("info.txt","w+");
    Scaledfile = fopen("vil.xls","w+");


FluxFile = fopen("condflux.xls","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();

    if (z==199)
    {
        //fprintf(Infofile,"Pulse Number: %d\n\n",z);
        fprintf(Infofile,"Applied Voltage = %f V\n\n\n",Vs);
        fprintf(Infofile,"Maximum Luminance = %.20lf W/cm2\n\n\n",max_lum*K);
        fprintf(Infofile,"Luminance per period = %.20lf W/cm2\n\n\n",tot_luminance*K*50E-9/5000E-6);
        fprintf(Infofile,"Maximum Current = %.20lf A/cm2\n\n\n",max_flux*1.6E-19);
        fprintf(Infofile,"Total Current = %.20lf A/cm2\n\n\n",totalflux*1.6E-19);
fprintf(Infofile,"Maximum Cathodic Electric Field = %f
V/cm\n\n\n",max_e_cathode);

fprintf(Infofile,"Maximum Anodic Electric Field = %f
V/cm\n\n\n",max_e_anode);

}

++z;

}

fclose(Scaledfile);

close(Infofile);

close(FluxFile);

return 0;
}

void write_scaled_file(void)
{
    max_lum = Lum[0];
    tot_luminance = 0;
    totalflux = 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] = e_anode[run_t]/max_e_anode;
}

for(run_t = 0;run_t<t+1;run_t++)
{
    Lum[run_t] = 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];
    }
}

Lum[run_t] = Lum[run_t]/max_lum;

max_lum = Lum[0];

for(run_t = 0;run_t<t+1;run_t++)
{
    if (max_lum<Lum[run_t])
    {
        max_lum = Lum[run_t];
    }
}

Lum[run_t] = Lum[run_t]/max_lum;

max_lum = Lum[0];

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

for(run_t = 0; run_t < t+1; run_t++)
{
    Vol[run_t] = 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++)
{
    totalflux = totalflux + Flu[run_t];
    Flu[run_t] = Flu[run_t]/max_flux;
}

max_flux_disp = 0;

for(run_t = 1; run_t < t+1; run_t++)
{
    fluxDisp = ((6.8624E-9)*((Vol[run_t] - Vol[run_t+1]))*max_v)/(q*delta_T);
    if (max_flux_disp < fluxDisp)
    {
        max_fluxdisp = fluxDisp;
    }
}
max_flux_disp = flux_disp;
}
}

max_flux_disp = max_flux_disp/max_flux;

if (((z==199)||(z==200))
{  
    for (run_t = 1;run_t<=1000;run_t++)
    {
        fprintf(Scaledfile,"%.5lf %.5lf %.5lf %.5lf %.5lf
",0.0,0.0,0.0,0.0,0.0);
    }
    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(Scaledfile,"%.5lf %.5lf %.5lf %.5lf %.5lf
",Vol[run_t-1],tot_flux_scaled,Lum[run_t],
e_cathode[run_t], e_anode[run_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(Scaledfile, "%.5lf %.5lf %.5lf %.5lf %.5lf\n", Vol[run_t], tot_flux_scaled, Lum[run_t],
e_cathode[run_t], e_anode[run_t]);

fprintf(FluxFile, "%.10lf\n", -Flu[run_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(Scaledfile, "%.5lf %.5lf %.5lf %.5lf %.5lf\n", -Vol[run_t], -tot_flux_scaled, Lum[run_t],
e_cathode[run_t], e_anode[run_t]);

fprintf(FluxFile, "%.10lf\n", Flu[run_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);
void driver(void) {
    int k;

    Vapp = 0;
    for(t_i=1;t_i<=(2*Ts);++t_i) {
        /* WRD: ctr_i is never referenced! */
        /*
        *  ctr_i = t_i;  */
        if( t_i <= RISE_TIME )               {
            Vapp += (Vs/RISE_TIME);
        }
        if((t_i>RISE_TIME) && (t_i<=FALL_TIME))
            {Vapp=Vs;
        }
        if( (t_i > FALL_TIME) && (t_i <= Ts) ) {
            Vapp -= (Vs/(Ts-FALL_TIME));
        }

        constants();
        cathodic_tunneling();
        bulk_phosphor();

        if (z==199)
        {
            Lt = 0;
        }
    }
}

fprintf(Scaledfile,"%.5lf %.5lf %.5lf
%.5lf %.5lf\n",-Vol[run_t],-tot_flux_scaled,Lum[run_t],
e_cathode[run_t], e_anode[run_t]);

fprintf(FluxFile,"%.10lf\n",-Flu[run_t]);
}
nahct = 0;
for (k = 1; k <= n; ++k) {
    Lt += (phos[k].Lit);
    nahct = nahct + phos[k].nah;
}
e_cathode[t] = phos[1].c3;
e_anode[t] = phos[n].c3;
Lum[t] = Lt;
Vol[t] = Vapp;
Flu[t] = phos[n].Fn;
t++;
}++j;
}

return;
}

void init (void)
{
    int k;

    for ( k=1; k<=n; ++k )
    {
        phos[k].nah = 0;
        phos[k].nt2 = 0;
        phos[k].nal = Nao-phos[k].nt2;
        phos[k].Fn = 0;
        phos[k].condnband = 0;
    }

    phos[0].Fn = 0;
    nc1 = 0.0*Neq;
    nc11 = Neq;
    nal = 0.0*Neq;
    nal1 = Neq;
    flux_disp = 0.6863E17;
}
return;
}

void cathodic_tunneling(void)
{
    double fld;
    double Pc1, Pc11, d1, d11;
    double f1, f11;
    
    fld = phos[1].c3;

    if(fld<0)
    {
        phos[0].Fn = 0;
    }
    else
    {
        register double quot; /* a temporary quotient */
        register double cc; /* a temporary constant */

        cc = (-b1) / (sqrt(m/m_star) * fld);
        d1 = cc * pow(E1, 1.5);
        d11 = cc * pow(E11, 1.5);
        cc = a1 * pow(m/m_star, 0.125) * pow(fld, 0.25);
        Pc1 = cc * pow(E1, 0.625) * exp(d1);
        Pc11 = cc * pow(E11, 0.625) * exp(d11);
        f1 = ncl1*Pc1;
        f11 = ncl11*Pc11;

        quot = ncl1 * (1.0/delta_T);
        f1 = (f1 > quot) ? quot : f1;

        quot = ncl11 * (1.0/delta_T);
        f11 = (f11> quot) ? quot : f11;

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

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

nc1 = nc1 - (f1 * delta_T);  
if (nc1<0)  
{
    f1 = f1 + nc1 * (1.0/delta_T);  
    nc1 = 0;  
}

nc11 = nc11 - (f11*delta_T);  
if (nc11<0)  
{
    f1 = f1 + nc11 * (1.0/delta_T);  
    nc11 = 0;  
}

phos[0].Fn = f1 + f11;  
if (set_tunnel==0)  
{
    if ((f1+f11)>1E16)  
    {
        fld_tunnel = phos[1].c3;
        set_tunnel = 1;
    }
}

return;
void forward_phosphor(void)
{
    register double fld;
    register double dnal, dnal, dnahdt, dnt2dt, dnah,
    register double sigma8;
    register double Prob3; /* a temporary variable refactored from
    Prob and Prob2; n
        * it could probably have a better name, but I
don't know what
        * it is for...
        */
    /* WRD: converted these variables from arrays to scalars.
        * because the array was never used as an array
        */
    register double R1, R2, R2A, R3, R4, R5, R8, R9, R12, R12A, R13;
    int k;

    for (k=1;k<=n;k++)
    {
        fld = phos[k].c3;
        fnew1 = 0.0;
        fnew2 = 0.0;
        fprimenew2 = 0.0;

        fld = fabs(fld);
        /* WRD: redundant (set above) */
        /* if (fld<(0.25E6))
            * fnew1, fnew2, and fprimenew2 should be zero, and were
already
            * set to zero above.
            */
        if ((fld>(0.25E6))&&f((f<((0.55E6))))
        {  
            /* WRD: fnew1 >= 0 because it is a square (and f >
            0.25E6) */


113
fnew1 = (fld*fld - fld*(2.0*0.25E6) + 
(0.25E6*0.25E6))*(1.0/(0.35E6*0.35E6));
}
else if ((fld>(0.55E6))&&(fld<(1.0E6))
{
    register double ff;
    /* WRD: what if (fld == 0.55E6) precisely? */
    ff = (fld*fld - fld * (2.0 * 0.55E6) + (0.55E6 * 
0.55E6))*(1.0/(0.35E6 * 0.35E6));
    /* fnew2 >= 0 and fprimenew2 >=0 because ff is a
square (and fld > 0.55E6) */
    fnew2 = 0.33 * ff;
    fprimenew2 = 0.67 * ff;
    fnew1 = 1.0 - (fnew2+fprimenew2);
    if (fnew1<0.0)
    {
        fnew1=0.0;
    }
}
else if (fld > 1.0E6)
{
    /* WRD: what if (fld == 1.0E6) precisely? */
    fnew2 = 0.33; 
    fprimenew2 = 0.67; 
}
phos[k].Lit = phos[k].nah * (B * Wx / TAU2);
phos[k].actcharge = Nao-phos[k].nal-phos[k].nah;
Prob3 = 3.14*radiu*radiu*(phos[k-1].Fn);
R1 = Prob3*fnew1*phos[k].nal;
R4 = phos[k].nah * (1.0/TAU2);
phos[k].nt2 = (phos[k].nt2 > Nt2) ? Nt2 : phos[k].nt2;
pt = Nt2-phos[k].nt2;
R2A = Prob3*fnew2*fnew3;
R2 = R2A * ((phos[k].nal <= pt) ? phos[k].nal : pt);
R12A = Prob3*fprimenew2*fprimenew3;
R12 = R12A * ((phos[k].nah <= pt) ? phos[k].nah : pt);
sigma8 = (fld > 1300000.0) ? 0.0 : (1.0/(delta_Tdipole));
R8 = sigma8 * ((phos[k].nt2 <= (Nao-phos[k].nal-phos[k].nah-phos[k].condnband)) ? phos[k].nt2 : (Nao-phos[k].nal-phos[k].nah-phos[k].condnband));
R3 = Prob3*fnew2*(1 - fnew3) * phos[k].nal;
R13 = Prob3*fprimenew2*(1-fprimenew3)*phos[k].nah;
R5 = 0.0;
R9 = 0.0;
// dtc = (-b1) * pow( ( m/m_star), -0.5) * pow(Etc, 1.5) * (1/fld);
// Ptc = a1 * pow( ( m/m_star), 0.125) * pow( Etc, 0.625) * pow(fld, 0.25) *exp(dtc);
      dnaldt = R4 - R1 - R2 - R3;
      dnahdt = R1 - R4 + R8 - R12 + R9 - R13 + R5;
      dnt2dt = R12 - R8 + R2;
      phos[k].Fn = phos[k-1].Fn + (R3 + R13 - R9)*Wx;
      dnt2 = dnt2dt * delta_T;
      phos[k].nt2 += dnt2;
      dnal = dnaldt * delta_T;
      phos[k].nal += dnal;
      dnah = dnahdt * delta_T;
      phos[k].nah += dnah;
      phos[k].condnband = (R3 + R13 - R9)*delta_T;
      total_charge = total_charge+(Nao-(phos[k].nal+phos[k].nah+phos[k].nt2)))*Wx;
}
flux_direction = 0;
anodic_interface();

void backward_phosphor(void)
{
    register double fld;
    register double dnaldt, dnal, dnahdt, dnt2dt, dnah ;
    register double sigma8;
    register double Prob3; /* a temporary variable refactored from Prob and Prob2;n

* it could probably have a better name, but I
don't know what
* it is for...
*/

/* WRD: converted these variables from arrays to scalars.
* because the array was never used as an array
*/
register double R1, R2, R2A, R3, R4, R5, R8, R9, R12, R12A, R13;

int k;

phos[n+1].Fn = phos[n].Fn;
for (k=n;k>=1;k--)
{
    fld = phos[k].c3;
    fnew1 = 0.0;
    fnew2 = 0.0;
    fprimenew2 = 0.0;

    fld = fabs(fld);
    if ((fld>(0.25E6))&&(fld<(0.55E6)))
    {
        fnew1 = (fld*fld - fld*(2.0*0.25E6) +
          (0.25E6*0.25E6))*(1.0/(0.35E6*0.35E6));
    }
    else if ((fld>(0.55E6))&&(fld<(1.0E6)))
    {
        register double ff;

        ff = (fld*fld - fld * (2.0 * 0.55E6) + (0.55E6 *
          0.55E6))*(1.0/(0.35E6 * 0.35E6));
        fnew2 = 0.33 * ff;
        fprimenew2 = 0.67 * ff;
        fnew1 = 1.0 - (fnew2+fprimenew2);
        if (fnew1<0.0)
        {
            fnew1=0.0;
        }
    }
else if (fld > 1.0E6)
{
    fnew2 = 0.33;
    fprimenew2 = 0.67;
}

phos[k].Lit = phos[k].nah * (B * Wx / TAU2);
phos[k].actcharge = Nao-phos[k].nal-phos[k].nah;
Prob3 = 3.14*radiu*radiu*(phos[k+1].Fn);
R1 = Prob3*fnew1*phos[k].nal;
R4 = phos[k].nah * (1.0/TAU2);
phos[k].nt2 = (phos[k].nt2 > Nt2) ? Nt2 : phos[k].nt2;
pt = Nt2-phos[k].nt2;
R2A = Prob3*fnew2*fnew3;
R2 = R2A * ((phos[k].nal <= pt) ? phos[k].nal : pt);
R12A = Prob3*fprimenew2*fprimenew3;
R12 = R12A * ((phos[k].nah <= pt) ? phos[k].nah : pt);
sigma8 = (fld > 1300000.0) ? 0.0 : (1.0/(delta_Tdipole));
R8 = sigma8 * ((phos[k].nt2 <= (Nao-phos[k].nal-
phos[k].nah-phos[k].condnband)) ?
    phos[k].nt2 : (Nao-phos[k].nal-phos[k].nah-
phos[k].condnband));
R3 = Prob3*fnew2*(1 - fnew3) * phos[k].nal;
R13 = Prob3*fprimenew2*(1-fprimenew3)*phos[k].nah;

/*

    if (((phos[k+1].Fn)/(fld*mobility)) > phos[k].actcharge)
    {
        R9 = ((phos[k+1].Fn)*sigma9)/(fld*mobility);
    }
else
    {
        R9 = phos[k].actcharge*sigma9;
    }
*/
R9 = 0.0;
R5 = ((phos[k+1].Fn*(1.0/Wx)) > phos[k].actcharge*(1.0/delta_T)) ? (phos[k].actcharge)*(1.0/delta_T) : phos[k+1].Fn*(1.0/Wx);

dnaldt = R4 - R1 - R2 - R3;
dnahdt = R1 - R4 + R8 - R12 + R9 - R13 + R5;
dnt2dt = R12 - R8 + R2;
phos[k].Fn = phos[k+1].Fn + (R3 + R13 - R9)*Wx;
dnt2 = dnt2dt * delta_T;
phos[k].nt2 += dnt2;
dnal = dnaldt * delta_T;
phos[k].nal += dnal;
dnah = dnahdt * delta_T;
phos[k].nah += dnah;
phos[k].condnband = (R3 + R13 - R9 - R5)*delta_T;
total_charge = total_charge+(Nao-
(phos[k].nal+phos[k].nah+phos[k].nt2))*Wx;

if (flux_direction == 0)
{
    flux_point = t_i;
}
flux_direction = 1;
cathodic_interface();

void bulk_phosphor(void)
{
    phos[n].Fn = 0.0;
total_charge = nc1+nc11+na1+na11;
if (phos[n].c3 < 0.0)
{
    anodic_tunneling();
}

if (phos[0].Fn>phos[n].Fn)
{
    forward_phosphor();
}
} 
else 
{ 
    backward_phosphor(); 
}

return;
}

void anodic_tunneling(void)
{

double fl1;

double Pa1,Pa11,d1,d11;

double f1,f11;

fld1 = phos[n].c3;

if(fld1>0.0)
{
    phos[n].Fn=0.0;
}
else
{
    register double cc; /* a temporary constant */

    fl1 = -fld1;
    cc = (-b2) / (fld1 * sqrt(m/m_star));
    d1 = cc * pow(E1, 1.5);
    d11 = cc * pow(E11,1.5);
    cc = a2 * pow( ( m/m_star), 0.125) * pow(fld1,0.25);
    Pa1 = cc * pow( E1, 0.625) * exp(d1);
    Pa11= cc * pow( E11, 0.625) * exp(d11);
    f1 = na1*Pa1;
    f11 = na11*Pa11;
    if(f1>na1/delta_T)
    {
        f1=na1/delta_T;
if (f1 > na1/delta_T)
{
    f1 = na1/delta_T;
}
if (f1 < 0.0)
{
    printf("f1<0 => Error in anodic interface \n");
    exit(0);
}
if (f11 < 0.0)
{
    printf("f11<0 => Error in anodic interface \n");
    exit(0);
}
phos[n].Fn = f1 + f11;
nal = nal - (f1*delta_T);
if (nal < 0.0)
{
    f1 = f1 + nal/delta_T;
    nal = 0.0;
}
nall = nall - (f11*delta_T);
if (nall < 0.0)
{
    f11 = f11 + nall/delta_T;
    nall = 0.0;
}
return;
}

void cathodic_interface()
{
    register double dnl1dt, dnll1dt, dnl_l1ldt;
}
dn1_11dt = ncl*Snd*Vth*(N11-ncl1);
dn1dt = phos[1].Fn-dn1_11dt;
dn11dt=dn1_11dt;
ncl = ncl + (dn1dt*delta_T);
if (ncl<0.0)
{
    ncl = ncl + (phos[1].Fn - dn1dt)*delta_T;
}
else
{
    ncl1 = ncl1 + (dn11dt*delta_T);
}

void anodic_interface()
{
    register double dn1dt,dn11dt,dn1_11dt;
    if (phos[n].Fn <0.0)
    {
        phos[n].Fn = - phos[n].Fn;
    }
    dn1_11dt = na1*Snd*Vth*(N11-na11);
dn1dt = phos[n].Fn-dn1_11dt;
dn11dt=dn1_11dt;
na1 = na1 + (dn1dt*delta_T);
if (na1<0.0)
{
    na1 = na1 + (phos[n].Fn - dn1dt)*delta_T;
}
else
{
    na11 = na11 + (dn11dt*delta_T);
}
}

void exchange(void)  {
    int k;
}
double temp1, temp11;

for( k = 0; k < n/2; ++k ) {
    phos[k+1].nal = phos[n-k].nal;
    phos[k+1].nah = phos[n-k].nah;
    phos[k+1].nt2 = phos[n-k].nt2;
    phos[k+1].Fn  = phos[n-k].Fn=0.0;
}

phos[0].Fn = 0.0;

temp1 = ncl;
ncl = nal;
nal = temp1;

temp11 = nc11;
nc11 = na11;
na11 = temp11;

return;
}

void constants(void) {
    register int k;
    register double A1, A2, A3, A4, A5, A6, A7;
    register double sum, sum1;
    register double activatorcharge;

    for( k=1; k<=n; ++k ) {
        activatorcharge = Nao-phos[k].nal-phos[k].nah;
        phos[k].spacecharge = activatorcharge - phos[k].nt2;
    }
    sum = 0.0;
    for( k=1; k<=n-1; ++k ) {
        sum += phos[k].spacecharge;
    }
    /* WRD: some of these variables are never initialized!! */
A1 = (q*W1*(1.0/ed)*(na1+ /*
na2+na3+na4+na5+na6+na7+na8+na9+na10+/*
na11-Neq));
A2 = ((W1*ez/ed) + n*Wx) * (q/ez) * (nc1+ /*
nc2+nc3+nc4+nc5+nc6+nc7+nc8+nc9+nc10+/*
nc11-Neq) ;
A3 = (q*Wx/W1/ed)*phos[n].spacecharge;
A4 = ( (q*Wx/Wx)/(2.0*ez) ) * (sum + phos[n].spacecharge) ;
A5 = ( (q*Wx)/ez ) * ( Wx + ((W1*ez)/ed) ) * sum ;
/*
sum1 = 0.0;
for( t=2; t<=(n-1); ++t) {
    sum2 = 0.0;
    for(k=1; k<=(t-1); ++k)
        sum2 += phos[k].spacecharge;
    sum1 += sum2;
}
*/
/* WRD: this is equivalent to the above and is much faster */
sum1 = 0.0;
for(k=1 ; k <= n-2 ; ++k) {
    sum1 += (n - (k+1)) * phos[k].spacecharge;
}

A6 = (q*Wx*Wx) * (1.0/(ez)) * sum1 ;
A7 = 2.0*W1 + ( ((n*Wx*ed)/ez) );
c1 = ( Vapp + A1 + A2 - A3 - A4 - A5 - A6 ) * (1.0/ A7) ;
phos[1].c3 = ( (ed * c1) - (q * (nc1 + /* nc2 +
nc3+nc4+nc5+nc6+nc7+nc8+nc9+nc10+/*
nc11 - Neq) ) ) * (1.0 / ez);
for(k=1; k<=(n-1); ++k) {
    phos[k+1].c3 = phos[k].c3 + (q*Wx/ez)*phos[k].spacecharge;
}

c5 = ( (ez*phos[n].c3) + (q*Wx* phos[n].spacecharge) - (q * (na1+ /* na2+na3+na4+na5+na6+na7+na8+na9+na10+ /*
nal1-Neq)) ) * (1.0 / ed);

return;
}
# include <stdio.h>

# include <math.h>

# include <string.h>

// Constants are defined here

# define l 2

# define k 8.62E-5

# define beta 0.25

# define s1 1E7

# define n1 1e19

// Variables are declared here

double T[1000];

double Et, Error1, ErrorS, ErrorSq;

double ErrorVal[1000];

double tes;
double maxI, maxIS, minErr;

char *op;

char *name;

int count, count1, e, i, j, gh, jPos;

double i1, i2, inte, integ, integ1, integ2, powup, pow1, IExp[1000],
ISim[1000][1000];

double ISimMinErr[1000];


/*****************************/

main ()
{

    // Read the temperature and experimental intensity values

    if ((TData = fopen("temperature.txt", "r")) == NULL)
    {
        fprintf(stderr, "Error opening temperature.txt file.\n");
        exit(1);
    }

    for (count=1; count<=700; count++)
    {
        fscanf(TData, "%lf\n", &T[count]);
    }

    fclose(TData);

    count--;
if ((ExpDataR = fopen("exp.txt", "r")) == NULL) {
    fprintf(stderr, "Error opening exp.txt file.\n");
    exit(1);
}

for (count1=1; count1<=700; count1++) {
    fscanf(ExpDataR, "%lf\n", &IExp[count1]);
}

fclose(ExpDataR);

// Open files for writing

if ( (ExpDataW = fopen("exp.xls", "w+")) == NULL) {
    fprintf(stderr, "Error opening file for writing experimental data.\n");
    exit(1);
}

for (count1=1; count1<=700; count1++) {
    fprintf(ExpDataW, "%20.1f\n", IExp[count1]);
}

if ( (ErrW= fopen("error.xls","w+")) == NULL) {
    fprintf(stderr, "Error opening file for writing mean square error data.\n");
    exit(1);
}

gh=0;
for (Et=0.01; Et<=0.5; Et=Et+0.01)
{
    gh++;
}

if ( (SimDataW = fopen("sim.xls","w+")) == NULL)
{
    fprintf(stderr, "Error opening file for writing theoretical
data.\n");

    exit(1);
}

// Run the loop through the temperature range in the ExpDataR file

e=0;

for (Et=0.01; Et<=0.5; Et=Et+0.01)
{
    e++;

    for(i = 1; i<=count; i++)
    {
        powup = (l/(l-1));

        // Read the experimental TSL intensity
        // Calculate the theoretical TSL intensity

        i1 = n*l*s1*exp(-Et/(k*T[i]));

        i2 = (l-1)*s1/beta;

        inte = T[i]*exp(-Et/(k*T[i]));

        integ = inte*((k*T[i]/Et)-
                2*pow((k*T[i]/Et),2)+6*pow((k*T[i]/Et),3));


integ2 = i2*integ;

integ1 = integ2 + 1;

pow1 = 1/pow(integ1,powup);

ISim[e][i] = i1*pow1;

}//Normalize Experimental Intensity

maxI = IExp[1];

for (j=1;j<=count;j++)
{
    if (maxI<=IExp[j])
    {
        maxI = IExp[j];
    }
}

for (j=1;j<=count;j++)
{
    IExp[j] = IExp[j]/maxI;
}

}//Normalize Theoretical Intensity

for (count1=1;count1<=e;count1++)
{
    maxIS = ISim[count1][1];

    for (j=1;j<=count;j++)
{ 
    if (maxIS<=ISim[count1][j])
    {
        maxIS = ISim[count1][j];
    }
}

for (j=1;j<=count;j++)
{
    ISim[count1][j] = ISim[count1][j]/maxIS;
}

//Calculate the mean squared error
for (j=1;j<=e;j++)
{
    ErrorSq = 0;

    for (i = 1; i<=count;i++)
    {
        Error1 = ISim[j][i] - IExp[i];

        ErrorS = pow(Error1,2);

        ErrorSq = ErrorSq + ErrorS;
    }

    ErrorSq = pow(ErrorSq,0.5);
    ErrorSq = ErrorSq/count;
    ErrorVal[j] = ErrorSq;

    fprintf(ErrW,"%.2lf %.10lf\n",j*0.01,ErrorSq);
fclose(ExpDataR);
fclose(ExpDataW);
fclose(ErrW);

minErr = ErrorVal[1];

for (j=2;j<=e;j++)
{
    if (minErr/ErrorVal[j])
    {
        minErr=ErrorVal[j];

        jPos = j;
    }
}

Et = jPos*0.01;

printf("Depth of trap level = %.3lf eV\n",Et);
printf("Escape frequency = %.3lf /second\n",s1);
printf("Order of process = %d\n",l);

for(i = 1; i<=count; i++)
{
    // Calculate the theoretical TSL intensity

    powup = (l/(l-1));

    i1 = n1*s1*exp(-Et/(k*T[i]));

    i2 = (l-1)*s1/beta;

    inte = T[i]*exp(-Et/(k*T[i]));
\[
\text{integ} = \text{inte} * ((k * T[i] / Et) - 2^{\text{pow}((k * T[i] / Et), 2)} + 6^{\text{pow}((k * T[i] / Et), 3)}); \\
\text{integ2} = i2 * \text{integ}; \\
\text{integ1} = \text{integ2} + 1; \\
\text{pow1} = 1 / \text{pow(integ1, powup)}; \\
\text{ISimMinErr[i]} = i1^{\text{pow1}};
\]

//Normalize Theoretical Intensity

\text{maxIS} = \text{ISimMinErr[1]};

\text{for (i=2; i<=count; i++)}
{ 
    \text{if (maxIS<=ISimMinErr[i])}
    { 
        \text{maxIS} = \text{ISimMinErr[i]};
    }
}

\text{for (i=1; i<=count; i++)}
{ 
    \text{ISimMinErr[i]} = \text{ISimMinErr[i]} / \text{maxIS};
}

\text{for(i = 1; i<=count; i++)}
{ 
    \text{fprintf(SimDataW, "%.3lf %.20lf %.20lf\n", T[i], IExp[i], ISimMinErr[i]);}
}

\text{fclose(SimDataW);}
References


Vita

Praveen Kumar Sivakumar, was born to Sivakumar Ramachandran and Vijayalakshmi Sivakumar, on January 9, 1979, in Chennai, India. He earned his Bachelors in Electronics and Communication Engineering from University of Madras in May 2000. He worked as Research Assistant in the Electronic Devices Research Lab at University of Kentucky until May 2006. He is currently working as Test Engineer at Creation Technologies, Lexington.