# MODELING OF LEDS WITH SILVACO

DRAGICA VASILESKA

### OUTLINE

- Introductory Concepts
- Example 1: Single Quantum Well Blue GaN LED
- Example 2: Multiple Quantum Well UV LED

# INTRODUCTORY CONCEPTS

### SINGLE AND MULTIPLE QUANTUM WELL STRUCTURES

A QW is synthesized from two different semiconductors. Consider two semiconductors with bandgap  $E_{g, \text{ barrier}}$  and  $E_{g, \text{ well}}$ . If the band alignment is straddled, the following QW band diagram is obtained:



- If L<sub>QW</sub> is large, quasi-3D behavior is obtained. Size quantization is then negligibly small.
- If L<sub>QW</sub> is sufficiently small, size quantization occurs.
- Absorption edge of the structure:

 $E_{g, QW} = E_{g, well} + E_{0, e} + E_{0, h}$ 

... where  $E_{0, e}$  is quantized electron energy ... where  $E_{0, h}$  is quantized hole energy

- Emission energy =  $E_{g, QW} = hv$
- The emission energy of the QW is different from either bandgap energy of the two semiconductors. Thus, a new synthetic material has been formed that is only remotely related to the bulk materials it is made of. This is why QWs are exciting materials.

#### Advantages of QW structures

Why are QW structures advantageous?

- Freedom to design transition energies
- High radiative efficiency. QW structures have a small volume. Therefore, when carriers are injected into a QW structure, the free carrier concentration in a QW is high. At high free carrier concentrations, non-radiative deep-level transitions are less likely. (Why?) QW structures therefore have high radiative efficiency.
- Low laser thresholds. Due to the small volume, the carrier density required to achieve population inversion is small. Therefore the threshold current density of QW structures is low.
- Surface recombination. Surface recombination is less important in QW structures as compared to bulk material. In QW structures, carriers are trapped by the QW and, therefore, cannot reach the surface. This is shown in the following figure:



- AlGaAs / GaAs is a frequently used QW system
- AlGaAs / GaAs is lattice matched for all Al compositions to the GaAs substrates
- Luminescence emission measurements allow one to determine the energy shift due to the quantum size effect. The following graph shows experimental QW emission energies versus QW thickness:





## **PROPERTIES OF 2DEGS**

Heterojunction Type	μ <sub>0</sub> , cm²/Vs	n <sub>s</sub> , cm <sup>-2</sup>	⊿E <sub>G</sub> , eV	⊿E <sub>c</sub> , eV
Al <sub>0.3</sub> Ga <sub>0.7</sub> As/GaAs	5400	<b>1.4 x 10</b> <sup>12</sup>	0.38	0.22
Al <sub>0.3</sub> Ga <sub>0.7</sub> As/In <sub>0.2</sub> Ga <sub>0.8</sub> As	6400	<b>2.2 x 10</b> <sup>12</sup>	0.58	0.41
In <sub>0.52</sub> Al <sub>0.48</sub> As/In <sub>0.53</sub> Ga <sub>0.47</sub> As	10 000	<b>3.0 x 10</b> <sup>12</sup>	0.71	0.52
Al <sub>0.3</sub> Ga <sub>0.7</sub> N/GaN	1 400	<b>1.3 x 10</b> <sup>13</sup>	0.6	0.42

III-V heterostructures: - more In in the channel layer leads to higher mobility  $\mu_0$ - larger  $\Delta E_{\rm C}$  causes a higher higher sheet concentration  $n_{\rm S}$ 

AIGaN/GaN:

- lower mobility than III-V's
- rather moderate  $\Delta E_{\rm C}$  but extremely high  $n_{\rm S}$  WHY ?

#### 2DEGs in AIGaN/GaN Structures

Ν

Ga

- Electronegativity polar nature of the bonds in AlGaN and GaN
- Deviation of the GaN and AlGaN crystal structure from the ideal structure: spontaneous polarization
- Different spontaneous polarizations in AlGaN and GaN gradient of the polarization at the interface
- Difference in the lattice constants in AlGaN and GaN strained AlGaN additional polarisation component: piezoelectric polarization

#### 2DEGs in AlGaN/GaN Structures



At the AlGaN/GaNinterface occurs a positive net charge +  $\sigma$  leading to the formation of a 2DEG in the GaN.

Two important messages:

- Only a small portion of the 2DEG electrons is caused by the barrier doping !
- Even without any doping very high 2DEG sheet concentrations are possible!



#### 2DEGs in AIGaN/GaN Structures



Measured 2DEG sheet concentration *n*<sub>S</sub> in Al<sub>x</sub>Ga<sub>1-x</sub>N/GaN heterostructures vs. Al content *x* 



#### **Carrier Transport in 2DEGs**



#### 2DEG Low-Field Mobility in AIGaN/GaN vs. Sheet concentration

Note:  $\mu_0$  in GaN bulk (*n* = 10<sup>17</sup> cm<sup>-3</sup>) is about 700 cm<sup>2</sup>/Vs



#### Current blocking layers:

![](_page_16_Figure_1.jpeg)

AlGaN current-blocking layer in an AlGaN/GaN/GaInN multi-quantum well LED structure. (a) Band diagram without doping. (b) Band diagram with doping. The Al content in the electron-blocking layer is higher than in the p-type confinement layer.

#### Multiple quantum wells (MQW)

#### Band diagram:

![](_page_17_Figure_2.jpeg)

- A MQW structure has more than one well, that is more carriers can be accommodated.
- Single quantum well (SQW) structures have a problem: Band filling. If a QW is filled with carriers, luminescence saturation occurs at high current densities.

![](_page_18_Figure_0.jpeg)

![](_page_18_Figure_1.jpeg)

Solution: MQW structures:

![](_page_18_Figure_3.jpeg)

#### EXAMPLE 1 – SINGLE QUANTUM WELL BLUE GAN LED

## SILVACO PROGRAM INPUT DECK

```
go atlas
#
# 2 Core multi-thread simulation
#
# GaN LED Opto Device Simulation
# Silvaco International 2004, 2007
#
# Requires : ATLAS/BLAZE/QUANTUM/LED
# Blue single-quantum well LED
```

```
# Band offset
# dEc:dEv(GaN:InGaN)=0.7:0.3
# dEc:dEv(AlGaN:GaN)=0.7:0.3
#
```

#### # Parameter used for this blue SQW LED

# Epilayer # Material # Type # Thickness # Doping # Mobility #

 # p-Contact # GaN # p # 500 # 1e19 # 10 #

 # p-Emitter # Al0.2GaN # p # 100 # 1e19 # 10 #

 # Blue # In0.2GaN # - # 3 # - # 100 #

 # n-Contact # GaN # n # 4000 # 1e18 # 100 #

 # n-Buffer # GaN # - # 30 # - # 100 #

#----# SECTION 1 : MESH GENERATION
#----#
# 1 Dimensional Structure
# for A/cm^2 Unit
mesh width=1e8

```
x.mesh loc=0.0 spac=0.5
x.mesh loc=1.0 spac=0.5
#
y.mesh loc=0.0 spac=0.1
y.mesh loc=0.5 spac=0.001
y.mesh loc=0.55 spac=0.005
y.mesh loc=0.600 spac=0.0002
y.mesh loc=0.603 spac=0.0002
y.mesh loc=0.65 spac=0.005
y.mesh loc=5.00 spac=1.0
#
#-----
# SECTION 2: REGIONS AND ELECTRODES
#_____
region num=1 material=GaN y.max=0.5
region num=2 material=AIGaN y.min=0.5 y.max=0.6 x.comp=0.2
region num=3 material=InGaN y.min=0.6 y.max=0.603 x.comp=0.20 name=well \
   qwell led calc.strain polarization polar.scale=1.0 well.ny=50
region num=4 material=GaN y.min=0.603 substrate
#
electrode name=anode top
```

```
electrode name=cathode bottom
```

```
#-----
# SECTION 3: DOPING PROFILES
#-----
# p type is Mg
# n type is Si
doping region=1 uniform p.type conc=1e19
doping region=2 uniform p.type conc=1e19
doping region=4 uniform n.type conc=1e18
#
#-----
# SECTION 4: MATERIAL MODELS
#-----
#
material material=GaN taun0=1e-9 taup0=1e-9 copt=1.1e-8 \
   augn=1.0e-34 augp=1.0e-34
material material=AIGaN taun0=1e-9 taup0=1e-9 copt=1.1e-8 \
   augn=1.0e-34 augp=1.0e-34
material material=InGaN taun0=1e-9 taup0=1e-9 copt=1.1e-8 \
   augn=1.0e-34 augp=1.0e-34
#
```

```
# Lorentz Broaden factor
material well.gamma0=30e-3
#
material edb=0.080 eab=0.101
#
models k.p fermi incomplete consrh auger optr print
models region=3 k.p chuang spontaneous lorentz
#
mobility mun0=100 mup0=10
#
#-----
# SECTION 5: OUTPUT FLAGS and METHOD
#-----
#
output con.band val.band band.param charge polar.charge e.mobility \
   h.mobility u.srh u.radiative u.auger permi
#
method climit=1e-4 maxtrap=10
#
```

```
_____
# SECTION 6: INITIAL SOLUTION
#-----
#
solve init
solve prev
#
save outf=ledex01 1.str
#
#-----
# SECTION 7: BIAS RAMP and Save the SPECTRUM
#-----
#
probe name=Recombination integrate recomb
probe name=Radiative integrate radiative rname=well
#
log outf=ledex01.log
solve vstep=0.05 vfinal=3.5 name=anode
save outf=ledex01_3p5.str
save spectrum=ledex01_3p5.spc lmin=0.40 lmax=0.50 nsamp=100
```

```
solve vstep=0.05 vfinal=4.0 name=anode
save outf=ledex01_4p0.str
save spectrum=ledex01_4p0.spc lmin=0.40 lmax=0.50 nsamp=100
```

```
solve vstep=0.05 vfinal=5.0 name=anode
save outf=ledex01 5p0.str
save spectrum=ledex01_5p0.spc lmin=0.40 lmax=0.50 nsamp=100
#
#_____
# SECTION 8: PLOTTING CURVES
#-----
#
# V-I Curve
tonyplot ledex01.log -set ledex01_0.set
# I-L Curve
tonyplot ledex01.log -set ledex01_1.set
# EL Intensity at 3.5V, 4.0V and 5.0V
tonyplot -overlay ledex01_3p5.spc ledex01_4p0.spc ledex01_5p0.spc -set
ledex01 2.set
```

extract init infile="ledex01\_3p5.str" extract name="Electron" curve(depth,impurity="Electron Conc" material="All" \ x.val=0.5) outfile="ledex01\_3p5\_Electron.dat" extract name="Electron" curve(depth,impurity="Hole Conc" material="All" \ x.val=0.5) outfile="ledex01\_3p5\_Hole.dat"

```
extract init infile="ledex01_4p0.str"
extract name="Electron" curve(depth,impurity="Electron Conc" material="All" \
x.val=0.5) outfile="ledex01_4p0_Electron.dat"
extract name="Electron" curve(depth,impurity="Hole Conc" material="All" \
x.val=0.5) outfile="ledex01_4p0_Hole.dat"
```

```
extract init infile="ledex01_5p0.str"
extract name="Electron" curve(depth,impurity="Electron Conc" material="All" \
x.val=0.5) outfile="ledex01_5p0_Electron.dat"
extract name="Electron" curve(depth,impurity="Hole Conc" material="All" \
x.val=0.5) outfile="ledex01_5p0_Hole.dat"
```

tonyplot -overlay ledex01\_3p5\_Electron.dat ledex01\_3p5\_Hole.dat ledex01\_4p0\_Electron.dat ledex01\_4p0\_Hole.dat ledex01\_5p0\_Electron.dat ledex01\_5p0\_Hole.dat -set ledex01\_3.set quit

#### CHARACTERISTIC SILVACO STATEMENTS

- Strain definition → REGION STATEMENT
   CALC.STRAIN, POLAR.SCALE, POLARIZATION
- Broadening → LORENTZ, CHUANG, SPONTANEOUS
- k.p model → BAND PARAMETERS
- To get the photoluminescence spectra → QWELL and LED have to be specified under the region statement

![](_page_29_Figure_0.jpeg)

![](_page_30_Figure_0.jpeg)

![](_page_31_Figure_0.jpeg)

![](_page_32_Figure_0.jpeg)

Depth ()

# EXAMPLE 2 – MULTIPLE QUANTUM WELL UV LED

![](_page_34_Figure_0.jpeg)

![](_page_35_Figure_0.jpeg)

![](_page_36_Figure_0.jpeg)

Electron and Hole Conc. at Anode Voltage=3.5V

![](_page_37_Figure_1.jpeg)

Depth ()

Electron and Hole Conc. at Anode Voltage=4.0V

![](_page_38_Figure_1.jpeg)

Electron and Hole Conc. at Anode Voltage=5.0V

![](_page_39_Figure_1.jpeg)

# SELF-HEATING EFFECTS IN LEDS

## OUTLINE

- Modeling self-heating effects with Silvaco
- Example 3: Self-heating effects in LEDs

## MODELING SELF-HEATING EFFECTS WITH SILVACO

DRAGICA VASILESKA

### **IS SELF-HEATING IMPORTANT?**

#### **Power Density Extrapolation**

![](_page_43_Figure_2.jpeg)

#### **HEATING VS. DEVICE PERFORMANCE**

- In most cases heat degrades device performance because it degrades carrier mobility and, therefore, the on-state current, i.e. the transistor drive.
- Heating is severely degrading mechanism in SOI device technology due to the low thermal conductivity of the underlying SiO<sub>2</sub> box layer.
- In both conventional MOSFET devices and SOI devices heating increases the breakdown voltage of the transistor.
- Heating is most simplistically modeled with a Fourier law.

#### APPROXIMATIONS MADE IN SILVACO

- Low field transport =>
  - Electron temperature equals the lattice temperature (no self-heating)
  - Dominant scattering mechanism at low electric fields is acoustic phonon scattering (isotropic, therefore very effective in randomization of the mobility)
  - Energy balance equation for acoustic phonons reduces to simple Joule heating conduction equation

## LATTICE HEATING – FOURIER LAW

![](_page_46_Figure_1.jpeg)

## SPECIFIC THERMAL ENERGY VS. TEMPERATURE

$$\frac{\partial e}{\partial t} = c \frac{\partial T}{\partial t} \tag{4}$$

where c = c(x, t) is the thermal capacity  $\left| \frac{J}{\lg K} \right|$ .

- The thermal capacity is also called specific heat capacity (or simply, specific heat).
- It describes the ability of a material to store the heat and refers to the quantity that represents the amount of heat required to change the temperature of one unit of mass by one degree.

![](_page_47_Picture_5.jpeg)

## DERIVATION OF THE HEAT DIFFUSION EQUATION

![](_page_48_Figure_1.jpeg)

### HEAT DIFFUSION EQUATION

#### 1<sup>st</sup> law (energy conservation) $\rightarrow$

Heat conduction = Rate of change of energy storage

$$k\frac{\partial^2 T}{\partial^2 x} = C\frac{\partial T}{\partial t}$$

Specific heat

•Conditions:

 $t >> \tau \equiv$  scattering mean free time of energy carriers  $L >> l \equiv$  scattering mean free path of energy carriers

•Breaks down for applications involving thermal transport in small length/ time scales, e.g. nanoelectronics, nanostructures, NEMS, ultrafast laser materials processing... Theoretical Models implemented in Silvaco ATLAS Device Simulator

![](_page_50_Picture_1.jpeg)

I emperature dependent mobilities and diffusion coefficients

### ANALOGY TO ELECTRICAL VARIABLES

$$q = kA \frac{T_1 - T_2}{L} = \frac{T_1 - T_2}{(L/kA)}$$

![](_page_51_Figure_2.jpeg)

#### ENERGY TRANSFER BETWEEN THE ELECTRON BATH AND THE PHONON BATH

![](_page_52_Figure_1.jpeg)

## ASU APPROACH TO THERMAL MODELING

$$\left( \frac{\partial}{\partial t} + v_e(\mathbf{k}) \cdot \nabla_r + \frac{e}{\hbar} E(\mathbf{r}) \cdot \nabla_k \right) f = \sum_{\mathbf{q}} \left\{ W_{e,\mathbf{q}}^{\mathbf{k}+\mathbf{q}\to\mathbf{k}} + W_{a,-\mathbf{q}}^{\mathbf{k}+\mathbf{q}\to\mathbf{k}} - W_{e,-\mathbf{q}}^{\mathbf{k}\to\mathbf{k}+\mathbf{q}} - W_{a,\mathbf{q}}^{\mathbf{k}\to\mathbf{k}+\mathbf{q}} \right\}$$
$$\left( \frac{\partial}{\partial t} + v_p(q) \cdot \nabla_r \right) g = \sum_{\mathbf{k}} \left\{ W_{e,\mathbf{q}}^{\mathbf{k}+\mathbf{q}\to\mathbf{k}} - W_{a,\mathbf{q}}^{\mathbf{k}\to\mathbf{k}+\mathbf{q}} \right\} + \left( \frac{\partial g}{\partial t} \right)_{p-p}$$

J. Lai and A. Majumdar, "Concurent thermal and electrical modeling of submicrometer silicon devices", J. Appl. Phys., Vol. 79, 7353 (1996).

$$\begin{split} C_{LO} \frac{\partial T_{LO}}{\partial t} &= \frac{3nk_B}{2} \left( \frac{T_e - T_L}{\tau_{e-LO}} \right) + \frac{nm * v_d^2}{2\tau_{e-LO}} - C_{LO} \left( \frac{T_{LO} - T_A}{\tau_{LO-A}} \right), \\ C_A \frac{\partial T_A}{\partial t} &= \nabla \cdot \left( k_A \nabla T_A \right) + C_{LO} \left( \frac{T_{LO} - T_A}{\tau_{LO-A}} \right) + \frac{3nk_B}{2} \left( \frac{T_e - T_L}{\tau_{e-L}} \right). \end{split}$$

## VASILESKA CONTRIBUTION TO SILVACO MODEL

$$\kappa(z) = \kappa_0(T) \int_0^{\pi/2} \sin^3 \theta \left\{ 1 - \exp\left(-\frac{a}{2\lambda(T)\cos\theta}\right) \cosh\left(\frac{a - 2z}{2\lambda(T)\cos\theta}\right) \right\} d\theta$$

$$\lambda(T) = \lambda_0 (300/T)$$

$$\kappa_0(T) = \frac{135}{a+bT+cT^2} \quad \text{W/m/K}$$

• E. H. Sondheimer, "The Mean Free Path of Electrons in Metals", Advances in Physics, Vol. 1, no. 1, Jan. 1952, reprinted in Advances in Physics, Vol. 50, pp. 499-537, 2001.

 M. Asheghi,., M. N. Touzelbaev., K. E. Goodson, Y. K. Leung, and S. S. Wong., "Temperature Dependent Thermal Conductivity of Single-Crystal Silicon Layers in SOI Substrates," ASME Journal of Heat Transfer, Vol.120, pp. 30-33, 1998.

![](_page_54_Figure_6.jpeg)

### SIMULATION EXAMPLE: CONVENTIONAL MOSFET DEVICE

![](_page_55_Figure_1.jpeg)

## SIMULATION RESULTS: DD VS. ENERGY BALANCE

![](_page_56_Figure_1.jpeg)

### **OUTPUT CHARACTERISTICS**

![](_page_57_Figure_1.jpeg)

Thermal self-heating effects lead to a reduction of the *electron mobility* and *impact ionization rate* which, in turn, leads to smaller drain current.

### LATTICE TEMPERATURE

![](_page_58_Figure_1.jpeg)

## TOTAL HEAT POWER

![](_page_59_Figure_1.jpeg)

### INTRODUCTION OF LATTICE HEATING IN SILVACO

- Lattice heating is introduced in Silvaco in two places:
  - MODELS statement where one specifies lat.temp
  - Thermocontact

thermcontact num=1 x.min=0 x.max=1 y.min=0.799 \ y.max=0.802 alpha=3000

### MORE DETAILS

At least one thermal contact statement must be specified when simulating lattice heating effects

(MODELS LAT.TEMP). The THERMCONTACT statement must appear in the input deck before any METHOD statement.

**position** is a set of the position parameters described below. Either X.MIN, X.MAX, Y.MIN, and Y.MAX parameters are used to specify the exact postion of the contact or the ELEC.NUMBER parameter to specify an electrode number that the thermal contact coincides with..

**NUMBER** specifies a thermal contact number from 1 to 20. Contact numbers should be specified in increasing order. This parameters **must** be specified on all THERMCONTACT statements.

**ALPHA** specifies the reverse value of thermal resistance (a=1/RTH). This parameter may not be used if ELEC.NUMBER parameter has been specified.

#### MORE DETAILS ...

**EXT.TEMPER** specifies the external temperature. *Synonym*: TEMPERATURE

#### **Position Parameters**

**NAME** specifies which region the THERMCONTACT statement applies to. Note that the name must match the name specified in the NAME parameter of the REGION statement.

**DEVICE** specifies which device in MIXEDMODE simulation the THERMCONTACT statement applies to.

#### MORE DETAILS ...

#### Parameter Type Default Units

ALPHA Real W/(cm2·K) DEVICE Character ELEC.NUMBER Integer EXT.TEMPER Real 300 K NAME Character NUMBER Integer 1 X.MAX Real Right side of structure mm X.MIN Real Left side of structure mm Y.MAX Real Bottom of structure mm Y.MIN Real Top of structure mm Z.MIN Real Front microns Z.MAX Real Back microns

**ELEC.NUMBER** specifies an electrode number that the thermal contact is coincident with.

#### MORE DETAILS ...

#### **Coordinate Definition Example**

A thermal contact is located where y-coordinate values range from 10 mm to the bottom side of the structure and x-coordinate values range from the left edge of the structure to the right edge of the structure (be default). The external temperature is set to 300K and a thermal resistance of 1 is added.

Thus, the temperature at y = 10 um will be greater than 300K once lattice heating effects occur.

#### THERMCONTACT NUM=1 Y.MIN=10 EXT.TEMP=300 ALPHA=1

#### **Example Setting Thermal and Electrical Contacts Coincident**

The next statement line creates a thermal contact at the location of electrode #4. An external temperature of 400K is specified.

THERMCONTACT NUM=2 ELEC.NUM=4 EXT.TEMP=400

# EXAMPLE 3: SELF-HEATING EFFECTS IN LEDS

GAAS/ALGAAS BULK LED WITH SELF-HEATING EFFECT CYLRINDRICAL STRUCTURE LED SIMUALTION REQUIRE : DEVICE3D/GIGA3D

![](_page_66_Figure_0.jpeg)

![](_page_67_Figure_0.jpeg)

![](_page_68_Figure_0.jpeg)